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Analytic aspects of Borwein-type sign pattern problems

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Abstract

by Chen Wang

This dissertation consists of two articles proving two of the famous Borwein conjectures using analytic methods.

In the first article, I gave the historically first proof of the original Borwein Conjecture, namely the coefficients of the “Borwein polynomials" $(1-q)(1-q^2)(1-q^4)(1-q^5)\dots(1-q^{3n-2})(1-q^{3n-1})$ has a recurring sign pattern of $+--+--\dots$, based on specific expansions due to Andrews.

In the second article, the methods used in the first proof are generalized and refined to a much broader setting, enabling an improved proof of the original conjecture and the proof of the Second Borwein conjecture predicting the same patterns for the square of the Borwein polynomials, as well as a partial proof of my own conjecture that predicting the same patterns for the cube of the Borwein polynomials.

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List of notation

Thoughout the thesis

$(a_1, a_2, \cdots ; q)_n$	Shifted q-factorial defined by $\prod_l \prod_{k=1}^{n}(1 - a_l q^{k-1})$
$\begin{bmatrix} n \\ m \end{bmatrix}_q$	q-binomial defined by ... $P_n(q)$
The "Borwein Polynomial" $(q, q^2; q^3)_n$	
$Q_n(q)$	A general family of polynomials for which we want to estimate thei
$\gamma(s, a)$	Lower incomplete gamma function

1 Introduction

1.1 Motivation

1.1.1 The Borwein Conjecture

In 1990, Peter Borwein made the curious observation that the coefficients of

$$P_n(q) := \prod_{i=1}^{n}(1-q^{3i-2})(1-q^{3i-1}) = (q,q^2;q^3)_n$$

seems to have a repeating sign pattern of $+--$. Here we use the standard notation for q-shifted polynomials, namely

$$(a_1,a_2,\ldots,a_k;q)_n := \prod_{i=1}^{k}\prod_{j=0}^{n-1}(1-a_iq^j).$$

Equivalently, if we write

$$(q,q^2;q^3)_n = A_n(q^3) - qB_n(q^3) - q^2C_n(q^3) \tag{1.1}$$

then it appears that the polynomials A_n, B_n and C_n have nonnegative coefficients.

This observation is known as the *Borwein Conjecture*, and it first appeared in print in an 1995 paper by Andrews [And95]. Two closely related conjectures, dubbed the *Second* and *Third* Borwein conjectures, also appeared in [And95]. The Second Borwein conjecture states that the coefficients of $(q,q^2;q^3)_n^2$ also have a repeating sign pattern of $+--$. The Third Conjecture, a "mod 5" analogue of the First Conjecture, states that the coefficients of $(q,q^2,q^3,q^4;q^5)_n$ have a repeating sign pattern of $+----$. The author has observed in 2019 that a *cubic* version of the conjecture also appears to hold, namely the coefficients of $(q,q^2;q^3)_n^3$ has the same recurring pattern.

This cumulative thesis consists of two previously written papers. The historically first proof of the original Borwein Conjecture by the author is presented in Chapter 2. In Chapter 3, the author gave a unified framework for attacking similar sign-pattern problems, resulting in an "improved" proof of the First Borwein Conjecture as well as proofs of the Second Borwein Conjecture and (in a precise sense) "two thirds" of the Cubic Borwein Conjecture.

Both chapters are self-contained and can be read independently.

1.1.2 Related conjectures and prior results

These deceivingly simple conjectures intrigued many researchers after Andrews had introduced them to a larger audience. Various approaches were tried, mainly combinatorial, or using q-series

techniques (cf. e.g. [And95; Ber20b; BW05; Bre96; IKS99; SZ21; War01; War03; Zah06]).

Several further variations and generalisations to the conjecture were proposed (see [BS19; Bre96; IKS99]), with some of them directly inspired by the results in this thesis [SZ21; BD24]. We notice in particular Bressoud's conjecture in [Bre96], which stems from the following expansions in [And95]:

$$A_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j+1)/2} \begin{bmatrix} 2n \\ n+3j \end{bmatrix}_q, \tag{1.2}$$

$$B_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j-5)/2} \begin{bmatrix} 2n \\ n+3j-1 \end{bmatrix}_q, \tag{1.3}$$

$$C_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j+7)/2} \begin{bmatrix} 2n \\ n+3j+1 \end{bmatrix}_q, \tag{1.4}$$

These formulas are interesting because they belong to a larger family of polynomials, for which several sub-families have bijective and/or q-series related proofs of their non-negativity. Indeed, if we define

$$G(m,n,\alpha,\beta,K) := \sum_{j} (-1)^j q^{jK\frac{(\alpha+\beta)j+\alpha-\beta}{2}} \begin{bmatrix} m+n \\ n-Kj \end{bmatrix}_q, \tag{1.5}$$

where the q-binomial numbers are defined as

$$\begin{bmatrix} n \\ m \end{bmatrix}_q := \frac{(q;q)_n}{(q;q)_m (q;q)_{n-m}},$$

Then the polynomials A_n, B_n and C_n in Borwein's first conjecture can be written as

$$\begin{aligned} A_n(q) &= G(n,n,\tfrac{5}{3},\tfrac{4}{3},3), \\ B_n(q) &= G(n+1,n-1,\tfrac{2}{3},\tfrac{7}{3},3), \\ C_n(q) &= G(n-1,n+1,\tfrac{8}{3},\tfrac{1}{3},3). \end{aligned}$$

In the cases where α,β are non-negative integers that satisfy $1 \leqslant \alpha+\beta \leqslant 2K-1$ and $-K+\beta \leqslant n-m \leqslant K-\alpha$, the polynomials $G(m,n,\alpha,\beta,K)$ turns out to be the generating function of partitions contained in an $m \times n$ rectangle and satisfy so-called *hook-difference conditions* specified by α,β and K [Bre96]. Bressoud conjectured that $G(m,n,\alpha,\beta,K)$ are nonnegative for positive rational α,β where $\alpha K, \beta K \in \mathbb{Z}$ and the inequalities $1 \leqslant \alpha+\beta \leqslant 2K-1$ and $-K+\beta \leqslant n-m \leqslant K-\alpha$ hold. Several infinite families of these Bressoud polynomials with non-integer parameters have been proven to be nonnegative; unfortunately, the polynomials in the Borwein conjectures are not included in these results.

1.2 Contributions

It came as a pleasant surprise to the author that no attempt had been made from an analytical/asymptotic viewpoint, despite the fact that Andrews already stated in [And95] that such

an approach is likely to be viable. This statement is based on expansions [And95, (4.5)] for the polynomials A_n, B_n and C_n in ((1.1)), where the first terms of the expansions indeed have positive coefficients and appear to be asymptotically dominant. These expansion were pivotal in the first proof of the Borwein conjecture by the author (Chapter 2).

However, no such formula is known to exist for the second and third conjectures, nor for other variants of the conjecture. Instead, it turns out that similar asymptotic techniques can be applied directly to $P_n(q)$ and related polynomials. This of course introduces some further difficulties in the analysis — some of which we will elaborate below — but enables a uniform way to attack all the Borwein conjectures as well as additional variants (Chapter 3).

1.2.1 General strategy and tools

The main strategy used in the thesis in proving the Borwein conjectures is analytical in nature.

Let $\{Q_n(q)\}_{n\geqslant 1}$ be a family of palindromic polynomials (which can be the Borwein polynomial $P_n(q)$ and its powers in Chapter 3, or terms in the expansions of A_n, B_n and C_n in Section 2.3 of Chapter 2), then the coefficient $[q^m]Q_n(q)$ can be written as

$$\frac{1}{2\pi i}\int_\Gamma Q_n(q)\frac{dq}{q^{m+1}},$$

where Γ is any contour about 0 with winding number 1. We will choose Γ as a circle centred at 0 with radius r for some $r \in \mathbb{R}^+$, so that the integral becomes

$$[q^m]Q_n(q) = \frac{r^{-m}}{2\pi}\int_{-\pi}^{\pi} Q_n\left(re^{i\theta}\right)e^{-im\theta}\,d\theta. \tag{1.6}$$

We want to emphasise that, unlike the most common form of saddle point approximation in the textbooks, this is a two-parameter problem, since we are dealing with a family of polynomials. This proves to be the main difficulty we face in the estimation of the integral, since any inequality we use throughout the arguments needs to be good enough for the whole range of m.

1.2.2 Locating the saddle points

The next step is to choose an suitable radius $r = r(m,n)$ and estimate the integral in ((1.6)). Traditionally, we require the integration contour to pass through the saddle point(s) of the integrand $r^{-m}Q_n\left(re^{i\theta}\right)e^{-im\theta}$.

In our proof of the First Borwein conjecture in Chapter 2, the dominant saddle point is located on the positive real axis, and can be found as the minimum point of the real-valued function $r \mapsto r^{-m}Q_n(r)$ in $(0,1]$.

However, in Chapter 3, the dominant saddle points can no longer be found on the positive real axis; instead they are located near the third roots of unity. Here we choose r to be the minimum point of the real-valued function $r \mapsto r^{-m}\left|Q_n(r\exp(2\pi i/3))\right|$ in $(0,1]$. These are detailed in Sections 2.5 and 3.5.

1.2.3 The infinite cases

The radius r can be proved to be very close to 1 except for the first (and last) $O(n)$ coefficients of $Q_n(q)$. For those exceptional coefficients, we note that the first $O(n)$ coefficients of the polynomial $Q_n(q)$ agree with those of its infinite analogue $Q_\infty(q)$, and the infinite analogues have already established sign-pattern results, see Sections 2.4 and 3.3.

1.2.4 Estimation of the integrals

We choose a cut-off length θ_0 which depends on m and n (see Sections 2.7 and 3.6), and split the integral ((1.6)) into two parts: the parts that are within θ_0 of the saddle point locations (which is either 0 or $\pm 2\pi/3$) called the *peak*, and the rest called the *tail*. The integral of the peak(s) can be approximated by a Gaussian integral, and the tail integral can be bounded relative to the peak integral. These estimations comprise the main part of both proofs; see Sections 2.8, 2.9 and 3.8 for the peak estimations, and Sections 2.10, 2.11 and 3.9) for the tail bounds.

1.2.5 Computational verification

Finally, those estimations mentioned above only works for “sufficiently large" n. A lot works were done to tighten the relevant inequalities and improve the resulting lower bound of n, so that a direct verification of the conjectures below this lower bound becomes computationally feasible. For details of the computations we did, see Sections 2.13 and 3.10.

2

An analytic proof of the Borwein Conjecture

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Abstract

We provide a proof of the Borwein Conjecture, which states that the coefficients of $(q;q)_{3n}/(q^3;q^3)_n$ have a repeating sign pattern of $+--$, using analytic methods. The proof is done by utilizing an expansion by Andrews to extract the "main part" of the coefficients, and then bound the various "error terms" that arise from this expansion.

2.1 Introduction

In 1990, Peter Borwein observed that for an arbitrary non-negative integer n, the coefficients of the polynomial

$$\prod_{i=1}^{n}(1-q^{3i-2})(1-q^{3i-1})$$

have a repeating sign pattern of $+--$. A more formalized version appears in a 1995 paper by Andrews [And95]. Here, and in the sequel, we use the standard notation for q-shifted factorials,

$$(a;q)_n = (1-a)(1-aq)\cdots(1-aq^{n-1}), \text{ for } n \geqslant 1,$$
$$(a;q)_0 = 1.$$

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Conjecture 2.1.1 (P. BORWEIN) Let the polynomials $A_n(q)$, $B_n(q)$ and $C_n(q)$ be defined by the relationship

$$\frac{(q;q)_{3n}}{(q^3;q^3)_n} = A_n(q^3) - qB_n(q^3) - q^2C_n(q^3). \tag{2.1}$$

Then these polynomials have non-negative coefficients.

This statement is known as the *Borwein Conjecture*.

There have been many attempts to prove the Borwein Conjecture. Moreover, we find several variations and generalizations in the literature, see [And95; BW05; BS19; Bre96; War01; War03; Zah06], sometimes also conjecturally, sometimes with full or partial proofs. However, none of the proved variations and generalizations cover the original conjecture, Conjecture 2.1.1. It is fair to say that so far essentially two methods have been tried: bijective methods—such as in [Bre96; IKS99], and basic hypergeometric methods—such as in [And95; BW05; War03]. Surprisingly though, it seems that nobody has made an asymptotic attack on the conjecture. This may have to do with the fact that the "canonical" formulas for $A_n(q)$, $B_n(q)$ and $C_n(q)$, namely ((2.77))–((2.79)), are entirely unsuitable for asymptotic approximation, see the corresponding remarks in Section 2.14. Nonetheless, it turns out that there are formulas for $A_n(q)$, $B_n(q)$ and $C_n(q)$ that are amenable to asymptotics, which appear already in Andrews' paper [And95], where the original conjecture appears for the first time in print.

Theorem 2.1.2 (ANDREWS, [AND95, THEOREM 4.1]) *Let $A_n(q)$, $B_n(q)$ and $C_n(q)$ be defined as in ((2.1)). Then we have the expansions*

$$A_n(q) = \sum_{j=0}^{\lfloor n/3 \rfloor} \frac{q^{3j^2}(1-q^{2n})(q^3;q^3)_{n-j-1}(q;q)_{3j}}{(q;q)_{n-3j}(q^3;q^3)_{2j}(q^3;q^3)_j}, \tag{2.2}$$

$$B_n(q) = \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} \frac{q^{3j^2+3j}(1-q^{3j+2}+q^{n+1}-q^{n+3j+2})(q^3;q^3)_{n-j-1}(q;q)_{3j}}{(q;q)_{n-3j-1}(q^3;q^3)_{2j+1}(q^3;q^3)_j}, \tag{2.3}$$

$$C_n(q) = \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} \frac{q^{3j^2+3j}(1-q^{3j+1}+q^{n}-q^{n+3j+2})(q^3;q^3)_{n-j-1}(q;q)_{3j}}{(q;q)_{n-3j-1}(q^3;q^3)_{2j+1}(q^3;q^3)_j}. \tag{2.4}$$

As a matter of fact, after discussing these formulas briefly, Andrews says in [And95] that *"it might be possible to prove that $A_n(q)$ has positive coefficients by establishing sufficiently tight bounds on the coefficients that arise term-by-term in (4.5)"*, where Andrews' (4.5) is our ((2.2)).

In the present paper, we follow Andrews' advice. Our main discovery is that, in the sums ((2.2))–((2.4)), the first term, i.e., the term for $j = 0$, dominates all other terms. This makes these expressions superior to all other known expressions for the purpose of asymptotic estimations. We use analytic methods to bound the coefficients of $A_n(q)$, $B_n(q)$ and $C_n(q)$ away from 0 by expressing the coefficients as certain contour integrals and estimating these integrals. Section 2.2 contains the basic setting of our proof: it is explained how to break the contour integrals into a positive-valued main part and four error terms, thus reducing the Borwein Conjecture to the problem of obtaining sufficiently good upper bounds on the error terms.

After establishing some basic facts and fixing some parameters in Sections 2.3–2.7, we derive upper bounds for each of the error terms in Sections 2.8–2.11, which leads to a proof of the Borwein Conjecture for all $n > 7000$ in Section 2.12. Some auxiliary results of technical nature

are stated and proved separately in an appendix. The cases where $0 \leqslant n \leqslant 7000$ are directly verified by a computer calculation, see Section 2.13. We conclude our paper with Section 2.14, in which we recall in more detail the earlier mentioned variations and generalizations, and where we also comment on possible further implications of our analytic approach.

2.2 An outline of the proof

In this section, we provide a brief outline of our proof of the Borwein Conjecture.

First, we claim that non-negativity of the coefficients of $B_n(q)$ already implies the complete Borwein Conjecture. Indeed, we have

$$C_n(q) = q^{\deg B_n} B_n(1/q), \tag{2.5}$$

which proves the non-negativity of the coefficients of $C_n(q)$ given the non-negativity of the coefficients of $B_n(q)$. On the other hand, the elementary recursive formula [And95, Eq. (3.3)]

$$A_n(q) = (1 + q^{2n-1})A_{n-1}(q) + q^n(B_{n-1}(q) + C_{n-1}(q)) \tag{2.6}$$

allows us to get the non-negativity of the coefficients of $A_n(q)$ inductively from the non-negativity of the coefficients of $B_n(q)$ (and $C_n(q)$). Therefore, from now on, we will concentrate on $B_n(q)$.

In Section 2.3, we start by writing (see ((2.20)))

$$B_n(q) = \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} B_{n,j}(q),$$

where $B_{n,j}(q)$ is the j-th summand in the expansion ((2.3)). We then decompose $B_{n,j}(q)$ into the sum of two simpler polynomials, namely $D_{n,j}(q)$ and $E_{n,j}(q)$, see ((2.21)), ((2.22)), and ((2.23)), so that

$$B_{n,j}(q) = q(1 + q^n)D_{n,j}(q) + E_{n,j}(q).$$

The background of this decomposition is that the polynomials $D_{n,j}(q)$ and $E_{n,j}(q)$ are simpler to handle asymptotically. By summing over all j, we define

$$D_n(q) := \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} D_{n,j}(q), \qquad E_n(q) := \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} E_{n,j}(q),$$

so that

$$B_n(q) = q(1 + q^n)D_n(q) + E_n(q).$$

In particular, this decomposition shows that, to prove the non-negativity of the coefficients of $B_n(q)$, it suffices to prove the non-negativity of the coefficients of $D_n(q)$ and $E_n(q)$ separately. Some elementary properties about $D_n(q)$ and $E_n(q)$, including their degrees, are collected in Lemma 2.3.1. In particular, it turns out that $D_n(q)$ is a palindromic polynomial, that is, $D_n(q) = q^{\deg D_n} D_n(1/q)$, while $E_n(q)$ is not. The latter is the reason that, in the subsequent discussion, we also need the reciprocal polynomial of $E_n(q)$, that is, $F_n(q) = q^{\deg E_n} E_n(1/q)$.

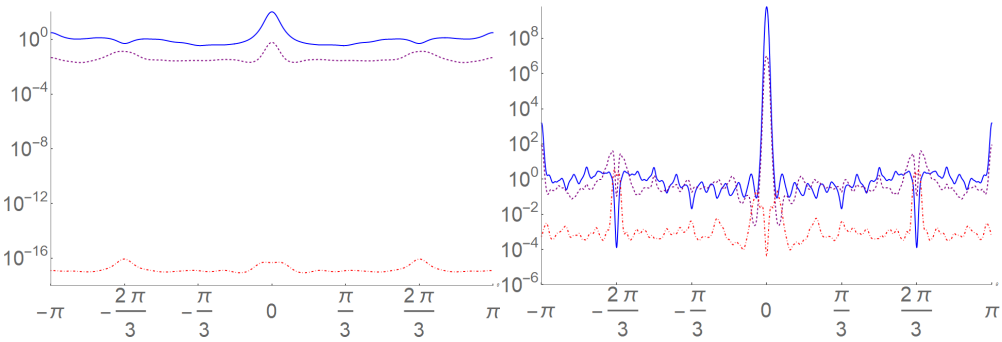

FIGURE 2.1: Modulus of $D_{36,0}(re^{i\theta})$ (solid), of $D_{36,2}(re^{i\theta})$ (dashed), and of $D_{36,8}(re^{i\theta})$ (dot-dashed). Left figure: $r = 0.836$, which is approximately the extremal value r_0 defined in ((2.34)). Right figure: $r = 0.97$. The vertical axes are in logarithmic scales.

The content of Section 2.4 is a proof of non-negativity of the coefficients of q^m in $D_n(q)$, $E_n(q)$ and $F_n(q)$ for $0 \leqslant m < n$. It relies on results of Andrews in [And95] and on a positivity result of Berkovich and Garvan from [BG05]. Thus, what remains to show, is non-negativity of the coefficients of q^m in $D_n(q)$ for $n \leqslant m \leqslant (\deg D_n)/2$, and an analogous result for $E_n(q)$ and for $F_n(q)$.

For notational simplicity, we will use the notations $P_n(q)$ and $P_{n,j}(q)$ throughout this paper to refer to multiple families of polynomials. For example, a proposition that is true for $P_n(q)$ for $P \in \{D, E, F\}$ means the proposition is true for all three families of polynomials $D_n(q)$, $E_n(q)$ and $F_n(q)$. We will also use the standard notation $[q^m]P_n(q)$ to represent the coefficient of q^m in the polynomial $P_n(q)$.

Using Cauchy's integral formula, the coefficient $[q^m]P_n(q)$ can be represented as the integral

$$\frac{1}{2\pi i}\int_\Gamma P_n(q)\frac{dq}{q^{m+1}},$$

where Γ is any contour about 0 with winding number 1. We will choose Γ as a circle centred at 0 with radius r for some $r \in \mathbb{R}^+$, so that the integral becomes

$$[q^m]P_n(q) = \frac{r^{-m}}{2\pi}\int_{-\pi}^{\pi} P_n\left(re^{i\theta}\right)e^{-im\theta}\,d\theta. \tag{2.7}$$

The exact choice of r is related to the *saddle point* of $q^{-m}P_{n,0}(q)$. We will elaborate on this in Section 2.5. The appropriate choice for r is a value smaller than 1 but close to 1, see Lemma 2.5.1.

We use the expansions $P_n(q) = \sum_j P_{n,j}(q)$ to write the integral ((2.7)) as

$$[q^m]P_n(q) = \sum_{j=0}^{\lfloor (n-1)/3\rfloor}\frac{r^{-m}}{2\pi}\int_{-\pi}^{\pi} P_{n,j}\left(re^{i\theta}\right)e^{-im\theta}\,d\theta. \tag{2.8}$$

Figure 2.1 illustrates the typical behaviour of $|D_{n,j}\left(re^{i\theta}\right)|$ on the circle $\{z \in \mathbb{C} \mid |z| = r\}$. In particular, we can observe the following general features in the graph:

- the terms with smaller j have a central peak at $\theta = 0$;
- the central peak of $|P_{n,j}\left(re^{i\theta}\right)|$ for small j looks like a translated-down version of the central peak for $|P_{n,0}\left(re^{i\theta}\right)|$. Since Figure 2.1 is on a logarithmic scale, this suggests that the magnitude $|P_{n,j}\left(re^{i\theta}\right)|$ could be controlled by a constant factor times $|P_{n,0}\left(re^{i\theta}\right)|$ in a neighbourhood of $\theta = 0$;
- for these terms, the values outside the small neighbourhood of $\theta = 0$ are very small compared to the peak value;
- when j becomes larger, the central peak disappears. However, it is apparent that the graph of $|P_{n,j}\left(re^{i\theta}\right)|$ for larger j (represented by the dot-dashed curve in the graph) is located in the lower part of the figure, indicating that $|P_{n,j}\left(re^{i\theta}\right)|$ could be controlled by a relatively small constant if j is large.

Based on these heuristics, we choose two cut-offs j_0 and θ_0 (to be determined in ((2.47)) and ((2.48))), and distinguish the following parts of the integrands $P_{n,j}\left(re^{i\theta}\right)e^{-im\theta}$, for $0 \leqslant j \leqslant (n-1)/3$:

- The term *primary peak* refers to the part where $j = 0$ and $|\theta| \leqslant \theta_0$.
- The term *secondary peaks* refers to the parts where $1 \leqslant j \leqslant j_0$ and $|\theta| \leqslant \theta_0$.
- The term *tails* refers to the parts where $0 \leqslant j \leqslant j_0$ and $\theta_0 < |\theta| \leqslant \pi$.
- Finally, the term *remainders* refers to the parts where $j > j_0$.

Naturally, the integral ((2.8)) can be divided into four sub-integrals corresponding to the four parts above.

For all $P \in \{D, E, F\}$, we make the following observations concerning the four sub-integrals:

- The primary peak can be approximated by a Gaußian integral. More specifically, if we define
$$g_P(n,r) = -\frac{\partial^2}{\partial\theta^2}\log P_{n,0}(re^{i\theta})\Big|_{\theta=0}, \tag{2.9}$$
then we should expect that
$$\int_{-\theta_0}^{\theta_0} P_{n,0}(re^{i\theta})e^{-im\theta}\,d\theta = P_{n,0}(r)\sqrt{\frac{2\pi}{g_P(n,r)}}(1+o(1)) \tag{2.10}$$
as $n \to \infty$.
- The secondary peaks will be bounded from above by a constant times the primary peak. We argue that
$$\begin{aligned}\left|\sum_{j=1}^{j_0}\int_{-\theta_0}^{\theta_0} P_{n,j}(re^{i\theta})e^{-im\theta}\,d\theta\right| &\leqslant \sum_{j=1}^{j_0}\int_{-\theta_0}^{\theta_0}\left|P_{n,j}(re^{i\theta})\right|\,d\theta \\ &\leqslant \sum_{j=1}^{j_0}\left(\sup_{|\theta|\leqslant\theta_0}\left|\frac{P_{n,j}\left(re^{i\theta}\right)}{P_{n,0}\left(re^{i\theta}\right)}\right|\right)\int_{-\theta_0}^{\theta_0}|P_{n,0}(re^{i\theta})|\,d\theta.\end{aligned} \tag{2.11}$$

- The tails will be estimated relative to its corresponding (primary or secondary) peak. More specifically, for $P \in \{D, E, F\}$, we will construct families of polynomials $\tilde{P}_{n,j}(r)$ with non-negative coefficients (see the paragraph before ((2.40))), acting as uniform upper bounds for $|P_{n,j}(re^{i\theta})|$ over the circle $\partial B(0,r) = \{z \in \mathbb{C} \mid |z| = r\}$, satisfying the relations

$$\begin{aligned} \tilde{P}_{n,0}(r) &= P_{n,0}(r), \\ \tilde{P}_{n,j}(|q|) &\geqslant |P_{n,j}(q)|, \end{aligned} \tag{2.12}$$

  for all $q \in \mathbb{C}$ and all $r \in \mathbb{R}^+$.

  With the help of $\tilde{P}_{n,j}(r)$, the tail integrals can be bounded above by

$$\begin{aligned} \left| \sum_{j=0}^{j_0} \int_{\theta_0}^{2\pi-\theta_0} P_{n,j}(re^{i\theta}) e^{-im\theta}\, d\theta \right| &\leqslant \sum_{j=0}^{j_0} \tilde{P}_{n,j}(r) \int_{\theta_0}^{2\pi-\theta_0} \left| \frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)} \right| d\theta \\ &\leqslant \left(\sum_{j=0}^{j_0} \frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)} \right) \left(\int_{\theta_0}^{2\pi-\theta_0} \sup_{0 \leqslant j \leqslant j_0} \left| \frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)} \right| d\theta \right) \times P_{n,0}(r). \end{aligned} \tag{2.13}$$

- The remainder will be directly controlled by the upper bounds $\tilde{P}_{n,j}(r)$. Namely, by ((2.12)), we have

$$\sum_{j=j_0+1}^{\lfloor (n-1)/3 \rfloor} \left| \int_{\pi}^{-\pi} P_{n,j}(re^{i\theta}) e^{-im\theta}\, d\theta \right| \leqslant \left(2\pi \sum_{j=j_0+1}^{\lfloor (n-1)/3 \rfloor} \frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)} \right) \times P_{n,0}(r). \tag{2.14}$$

Our next step is to estimate the relative error in the approximation ((2.10)), and to bound the other parts of the integral relative to the (presumably) dominating part $P_{n,0}(r)\sqrt{\frac{2\pi}{g_P(n,r)}}$. Based on ((2.10)) and the inequalities ((2.11)), ((2.13)) and ((2.14)), we give the following definitions in order to describe the error terms:

$$\epsilon_{0,P}(n,m,r) := \left| \frac{\sqrt{g_P(n,r)}}{\sqrt{2\pi} P_{n,0}(r)} \int_{-\theta_0}^{\theta_0} P_{n,0}(re^{i\theta}) e^{-im\theta}\, d\theta - 1 \right|, \tag{2.15}$$

$$\epsilon_{1,P}(n,r) := \left(\sum_{j=1}^{j_0} \sup_{|\theta|<\theta_0} \left| \frac{P_{n,j}\left(re^{i\theta}\right)}{P_{n,0}\left(re^{i\theta}\right)} \right| \right) \left(\sqrt{\frac{g_P(n,r)}{2\pi}} \int_{-\theta_0}^{\theta_0} \left| \frac{P_{n,0}(re^{i\theta})}{P_{n,0}(r)} \right| d\theta \right), \tag{2.16}$$

$$\epsilon_{2,P}(n,r) := \sqrt{\frac{g_P(n,r)}{2\pi}} \left(\sum_{j=0}^{j_0} \frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)} \right) \left(\int_{\theta_0}^{2\pi-\theta_0} \sup_{0 \leqslant j \leqslant j_0} \left| \frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)} \right| d\theta \right), \tag{2.17}$$

$$\epsilon_{3,P}(n,r) := \sqrt{2\pi g_P(n,r)} \sum_{j=j_0+1}^{\lfloor (n-1)/3 \rfloor} \frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)}. \tag{2.18}$$

It should be noted that only the first of these, $\epsilon_{0,P}(n,m,r)$, depends on m, namely the parameter which specifies the monomial q^m of which we are taking the coefficient in $P_n(q)$.

These definitions, along with the integral representation ((2.8)) and the inequalities ((2.11)), ((2.13)) and ((2.14)), imply that

$$[q^m]P_n(q) \geqslant \frac{P_{n,0}(r)}{r^m\sqrt{2\pi g_P(n,r)}}\left(1-\epsilon_{0,P}(n,m,r)-\epsilon_{1,P}(n,r)-\epsilon_{2,P}(n,r)-\epsilon_{3,P}(n,r)\right). \tag{2.19}$$

Once we have sufficiently good bounds on all these error terms so that their sum is smaller than 1, we can conclude that $[q^m]P_n(q)$ is indeed positive.

The primary peak error $\epsilon_{0,P}(n,m,r)$ is estimated in Section 2.8, the secondary peaks $\epsilon_{1,P}(n,r)$ are bounded in Section 2.9, Section 2.10 is devoted to bounding the remainders $\epsilon_{3,P}(n,r)$, and finally Section 2.11 treats the tails $\epsilon_{2,P}(n,r)$. All these estimations are valid for $n > 7000$ and $n \leqslant m \leqslant (\deg D_n)/2$ respectively $n \leqslant m \leqslant (\deg E_n)/2 = (\deg F_n)/2$, and their combination shows that the Borwein Conjecture holds for $n > 7000$, see Theorem 2.12.1 in Section 2.12. The cases where $n \leqslant 7000$ are disposed of by a (lengthy) computer calculation, the principles of which are explained in Section 2.13.

2.3 Decomposing $B_n(q)$

As we already explained in the introduction, the starting point of our proof of the Borwein Conjecture is Theorem 2.1.2, which provides certain expansions of the polynomials $A_n(q)$, $B_n(q)$ and $C_n(q)$. Based on the expansion ((2.3)), we define the family of polynomials $B_{n,j}(q)$ to be the summands in that expansion, so that

$$B_n(q) = \sum_{j=0}^{\lfloor (n-1)/3\rfloor} B_{n,j}(q). \tag{2.20}$$

The factor $(1-q^{3j+2}+q^{n+1}-q^{n+3j+2})$ in $B_{n,j}(q)$ turns out to be inconvenient, since our strategy is to bound quotients $B_{n,j}(q)/B_{n,j-1}(q)$ of successive terms. Therefore, we decompose it as

$$1-q^{3j+2}+q^{n+1}-q^{n+3j+2} = (1-q)+q(1+q^n)(1-q^{3j+1}).$$

This decomposition naturally extends to the family of polynomials $B_{n,j}(q)$ via the following definitions:

$$\begin{aligned} D_{n,j}(q) &:= \frac{(1-q^{3j+1})}{1-q^{3j+2}+q^{n+1}-q^{n+3j+2}}B_{n,j}(q) \\ &= \frac{q^{3j^2+3j}(q^3;q^3)_{n-j-1}(q;q)_{3j+1}}{(q;q)_{n-3j-1}(q^3;q^3)_{2j+1}(q^3;q^3)_j}, \end{aligned} \tag{2.21}$$

$$\begin{aligned} E_{n,j}(q) &:= \frac{1-q}{1-q^{3j+2}+q^{n+1}-q^{n+3j+2}}B_{n,j}(q) \\ &= \frac{q^{3j^2+3j}(1-q)(q^3;q^3)_{n-j-1}(q;q)_{3j}}{(q;q)_{n-3j-1}(q^3;q^3)_{2j+1}(q^3;q^3)_j}, \end{aligned} \tag{2.22}$$

so that

$$B_{n,j}(q) = q(1+q^n)D_{n,j}(q)+E_{n,j}(q). \tag{2.23}$$

By summing over all j, we define

$$D_n(q) := \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} D_{n,j}(q), \qquad E_n(q) := \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} E_{n,j}(q), \tag{2.24}$$

so that

$$B_n(q) = q(1+q^n)D_n(q) + E_n(q). \tag{2.25}$$

As we already indicated in the previous section, our estimations of the error terms $\epsilon_{0,P}(n,m,r)$ for $P \in \{D,E\}$ are only valid for $m \leqslant (\deg P_n)/2$, that is, only for "half of the coefficients", see Section 2.5, and in particular Lemma 2.5.1 to which we shall refer repeatedly. While this is fine for $D_n(q)$ — since $D_n(q)$ is palindromic, proving bounds for the first half of the coefficients automatically means to also have proved analogous bounds for "the second half" — this is a problem for $E_n(q)$ which is not palindromic. Here, we need to consider the reciprocal polynomial of $E_n(q)$, that is, $F_n(q) := q^{\deg E_n} E_n(1/q)$, and also prove estimations for $\epsilon_{i,F}$ as defined in ((2.15))–((2.18)). It is a routine calculation from ((2.24)) that with

$$F_{n,j}(q) := q^{3j} E_{n,j}(q) = \frac{q^{3j^2+6j}(1-q)(q^3;q^3)_{n-j-1}(q;q)_{3j}}{(q;q)_{n-3j-1}(q^3;q^3)_{2j+1}(q^3;q^3)_j} \tag{2.26}$$

we have

$$F_n(q) = \sum_{j=0}^{\lfloor (n-1)/3 \rfloor} F_{n,j}(q). \tag{2.27}$$

Remark: It is not hard to see that the functions $D_{n,j}(q)$, $E_{n,j}(q)$ and $F_{n,j}(q)$, as defined above, are actually polynomials for all j with $0 \leqslant j \leqslant \lfloor (n-2)/3 \rfloor$. (For a proof of this fact, see the factorizations ((2.36))–((2.39)) and the related discussions in Section 2.6.) However, in the special case $n \equiv 1 \pmod 3$ and $j = (n-1)/3$, ((2.21)), ((2.22)) and ((2.26)) fail to give polynomials. Thus, we restrict the domain of the definitions ((2.21)), ((2.22)) and ((2.26)) to $0 \leqslant j \leqslant \lfloor (n-2)/3 \rfloor$, and make alternative definitions in the "boundary case":

$$D_{3j+1,j}(q) := 0, \tag{2.28}$$

$$E_{3j+1,j}(q) := B_{3j+1,j}(q) = \frac{q^{3j^2+3j}(q;q)_{3j}}{(q^3;q^3)_j}, \tag{2.29}$$

$$F_{3j+1,j}(q) := q^{\deg E_{3j+1}} B_{3j+1,j}(1/q) = \frac{q^{3j^2-2}(q;q)_{3j}}{(q^3;q^3)_j}. \tag{2.30}$$

It is straightforward to see that, with these alternate definitions, and with the sums ((2.24)) and ((2.27)), we still have ((2.25)).

We collect some basic facts about these polynomials.

Lemma 2.3.1 *For $P \in \{D,E,F\}$, the polynomials $P_n(q)$ and $P_{n,0}(q)$ have the following properties:*

- *$D_n(q)$ is a palindromic polynomial, while $E_n(q)$ and $F_n(q)$ are reciprocal of each other. Therefore, it suffices to consider the coefficients $[q^m]P_n(q)$ for $0 \leqslant m \leqslant (\deg P_n)/2$.*

- $\deg D_n(q) = \deg E_n(q) = \deg F_n(q) = n^2-n-2$. *Furthermore, we have* $\deg P_{n,0}(q) = \deg P_n(q)$ *for all* $P \in \{D, E, F\}$.
- *The* $j = 0$ *terms in the expansions have a nice product form:*

$$D_{n,0}(q) = E_{n,0}(q) = F_{n,0}(q) = (1+q^2+q^4)(1+q^3+q^6)\cdots(1+q^{n-1}+q^{2n-2}). \quad (2.31)$$

- *The expression* ((2.31)) *implies the following formula for* $g_P(n,r)$ *as defined in* ((2.9)):

$$g_D(n,r) = g_E(n,r) = g_F(n,r) = \sum_{k=2}^{n-1} \frac{k^2 r^k (1+4r^k+r^{2k})}{(1+r^k+r^{2k})^2}. \quad (2.32)$$

2.4 The first n coefficients

In this section, we settle the non-negativity of the first n coefficients of $P_n(q)$ for $P \in \{D, E, F\}$ by considering the $n \to \infty$ limiting case.

To this end, we define

$$P_\infty(q) := \lim_{n\to\infty} P_n(q)$$

for all $P \in \{A, B, C, D, E, F\}$. The following lemma is a direct consequence of ((2.1)), ((2.21)), ((2.22)) and ((2.26)).

Lemma 2.4.1 *For all* $P \in \{A, B, C, D, E, F\}$ *and all* $n \geqslant 0$, *we have*

$$P_n(q) = P_\infty(q) + O(q^n).$$

This lemma says in particular that, for all $P \in \{D, E, F\}$, the non-negativity of $P_\infty(q)$ implies the non-negativity of $[q^m]P_n(q)$ for $m = 0, 1, \ldots, n-1$. The series $P_\infty(q)$, with $P \in \{D, E, F\}$ have indeed non-negative coefficients as we are going to show now. To this end, we first provide product formulas for $B_\infty(q)$ and $C_\infty(q)$.

Lemma 2.4.2 (Also see [And95, (4.3)–(4.4)]) *The power series* $B_\infty(q)$ *and* $C_\infty(q)$ *have the closed form expressions*

$$B_\infty(q) = \frac{(q^2, q^7, q^9; q^9)_\infty}{(q;q)_\infty}, \qquad C_\infty(q) = \frac{(q^1, q^8, q^9; q^9)_\infty}{(q;q)_\infty},$$

where we use the short notation

$$(a_1, a_2, \ldots, a_k; q)_\infty = (a_1;q)_\infty (a_2;q)_\infty \cdots (a_k;q)_\infty.$$

Proof: By Euler's pentagonal number theorem and the Jacobi triple product identity, we have

$$\begin{aligned}(q;q)_\infty &= \sum_{j\in\mathbb{Z}} (-1)^j q^{j(3j-1)/2} = \sum_{a=-1}^{1} \sum_{j\in\mathbb{Z}} (-1)^{3j+a} q^{(3j+a)(9j+3a-1)/2} \\ &= \sum_{a=-1}^{1} \sum_{j\in\mathbb{Z}} (-1)^{3j+a} q^{27\binom{j}{2}+(12+9a)j+a(3a-1)/2}\end{aligned}$$

$$= -q^2 \sum_{j\in\mathbb{Z}} (-1)^j q^{27\binom{j}{2}+3j} + \sum_{j\in\mathbb{Z}} (-1)^j q^{27\binom{j}{2}+12j} - q \sum_{j\in\mathbb{Z}} (-1)^j q^{27\binom{j}{2}+21j}$$
$$= -q^2(q^3, q^{24}, q^{27}; q^{27})_\infty + (q^{12}, q^{15}, q^{27}; q^{27})_\infty - q^2(q^{21}, q^6, q^{27}; q^{27})_\infty.$$

We compare this identity with the $n \to \infty$ limit of ((2.1)) to conclude the proof. □

We proceed to deduce non-negativity results for the power series $D_\infty(q)$, $E_\infty(q)$ and $F_\infty(q)$ from these forms. By taking the limit $n \to \infty$ in equations ((2.3)) and ((2.4)), and in ((2.21)), ((2.22)) and ((2.26)), we see that

$$\begin{aligned} D_\infty(q) &= C_\infty(q), \\ E_\infty(q) &= B_\infty(q) - qC_\infty(q) = (1-q)B_\infty(q) + q(B_\infty(q) - C_\infty(q)), \\ qF_\infty(q) &= B_\infty(q) - C_\infty(q). \end{aligned}$$

An immediate conclusion is that $D_\infty(q)$ also has non-negative coefficients. In order to prove analogous results for $E_\infty(q)$ and $F_\infty(q)$, it suffices to show that $B_\infty(q) - C_\infty(q)$ has non-negative coefficients. To prove this claim, we invoke Gordon's Partition Theorem.

Theorem 2.4.3 (GORDON, [GOR61]) *Let $k \in \mathbb{Z}^+$ and $1 \leqslant i \leqslant k$. Then the q-series*

$$G_{k,i}(q) := \frac{(q^i, q^{2k+1-i}, q^{2k+1}; q^{2k+1})_\infty}{(q,q)_\infty}$$

is the generating function for partitions in which 1 appears no more than $i-1$ times and any two consecutive integers appears no more than $k-1$ times in total.

As a consequence, each coefficient of $G_{k,i}(q)$ is increasing with respect to i, and by Lemma 2.4.2 we have $B_\infty(q) - C_\infty(q) = G_{4,2}(q) - G_{4,1}(q)$.

Thus we have proved that $P_\infty(q)$ has non-negative coefficients for $P \in \{D, E, F\}$. Combined with Lemma 2.4.1, we have the following result concerning the first n coefficients of $P_n(q)$.

Theorem 2.4.4 *For all $n \geqslant 1$, $0 \leqslant m \leqslant n-1$, and all $P \in \{D, E, F\}$, we have*

$$[q^m]P_n(q) \geqslant 0.$$

2.5 Locating the saddle point

The results of the last section show that it suffices to consider $[q^m]P_n(q)$ for $m \in [n, (\deg P_n)/2]$. The purpose of this section is to describe our choice of the radius r in ((2.7)), under the above restriction on m.

The method that we apply is a saddle point analysis of the function $z \mapsto z^{-m}P_{n,0}(z)$ (cf. [FS09, Chapter VIII] and [Won89, Section II.4]). Our choice of the radius r will be a saddle point of the function $z \mapsto z^{-m}P_{n,0}(z)$. It turns out that there is a unique saddle point on the positive real axis, and we have very tight bounds on the position of this point under the condition $m \in [n, (\deg P_n)/2]$. These results will be proved in the following lemma. They are vital in our estimations of the error terms $\epsilon_{i,P}$ in Sections 2.8–2.11.

Lemma 2.5.1 *For all $P \in \{D, E, F\}$, all integers $n \geqslant 1$, and $m \in (0, \deg P_n)$, the equation*

$$\frac{d}{dr}\left(r^{-m} P_{n,0}(r)\right) = 0 \tag{2.33}$$

has a unique solution $r_s \in \mathbb{R}^+$. Moreover, if $n \leqslant m \leqslant (\deg P_n)/2$, then we have $r_0 < r_s \leqslant 1$ where

$$r_0 = e^{-\sqrt{\alpha/n}}, \tag{2.34}$$

and $\alpha = 2/\sqrt{3}$ is the maximum value of the function $x \mapsto \frac{1+2x}{1+x+x^2}$ on $[0, 1]$.
Proof: The equation ((2.33)) can be transformed into

$$\frac{r P'_{n,0}(r)}{P_{n,0}(r)} = m.$$

Let us write $f_{n,P}(r)$ for the left-hand side. From the definition of the polynomials $P_{n,0}$ in ((2.31)), we have

$$f_{n,D}(r) = f_{n,E}(r) = f_{n,F}(r) = \sum_{k=2}^{n-1} \frac{k(2r^{2k} + r^k)}{1 + r^k + r^{2k}}.$$

These functions attain the special values

$$f_{n,P}(0) = 0, \qquad f_{n,P}(1) = (\deg P_n)/2, \qquad \lim_{r \to +\infty} f_{n,P}(r) = \deg P_n. \tag{2.35}$$

Moreover, all $f_{n,P}(r)$ are increasing functions in $\mathbb{R}^+$ since we have

$$\frac{d}{dr} \frac{2r^{2k} + r^k}{1 + r^k + r^{2k}} = \frac{kr^{k-1}(1 + 4r^k + r^{2k})}{(1 + r^k + r^{2k})^2} > 0.$$

The existence and uniqueness of solution follows immediately.

It remains to prove the bounds on r. Since $f_{n,P}(r)$ is increasing, it suffices to show that $f_{n,P}(r_0) < n$ and $f_{n,P}(1) \geqslant (\deg P_n)/2$. The latter is true due to the second equation in ((2.35)). In order to see the former inequality, we argue as follows:

$$\begin{aligned} f_{n,P}(r_0) &< \sum_{k=1}^{n} \frac{k(2r_0^{2k} + r_0^k)}{1 + r_0^k + r_0^{2k}} < \sum_{k=1}^{n} \alpha k r_0^k < \alpha \sum_{k=1}^{\infty} k r_0^k \\ &= \alpha \frac{r_0}{(1 - r_0)^2} < \alpha (\log r_0)^{-2} = n. \end{aligned}$$

□

2.6 The auxiliary polynomials $\tilde{P}_{n,j}(r)$

As mentioned in Section 2.2, we will construct families of polynomials $\tilde{P}_{n,j}(r)$ satisfying ((2.12)). These polynomials provide upper bounds for $|P_{n,j}(re^{i\theta})|$ with respect to θ. On the way, we also show that $D_{n,j}(q)$, $E_{n,j}(q)$ and $F_{n,j}(q)$ are polynomials in q, as claimed in Remark 1.

To this end, we first note that the inequality $|f(re^{i\theta})| \leqslant f(r)$ trivially holds if f is a polynomial with non-negative coefficients. Therefore, we proceed to factor out such parts from the polynomials $P_{n,j}(q)$, and bound the cofactor from above by the triangle inequality. Due to the relationship $F_{n,j}(q) = q^{3j}E_{n,j}(q)$, we will only explicitly write the factorization results for $P \in \{D, E\}$.

Using the definitions ((2.21)) and ((2.22)), we arrive at the factorizations

$$D_{n,j}(q) = \left(\frac{q^{3j^2+3j}(q^3;q^3)_{n-3j}(q;q)_{3j+1}}{(q^3;q^3)_{3j+1}(q;q)_{n-3j}}\begin{bmatrix}3j+1\\ j\end{bmatrix}_{q^3}\right)\left(\frac{(q^3;q^3)_{n-j-1}}{(q^3;q^3)_{n-3j-1}}\right), \tag{2.36}$$

$$E_{n,j}(q) = \left(\frac{q^{3j^2+3j}(q^3;q^3)_{n-3j}(q;q)_{3j+1}(1-q^3)}{(q^3;q^3)_{3j+1}(q;q)_{n-3j}(1-q^{9j+3})}\begin{bmatrix}3j+1\\ j\end{bmatrix}_{q^3}\right)\left(\frac{1+q^{3j+1}+q^{6j+2}}{1+q+q^2}\frac{(q^3;q^3)_{n-j-1}}{(q^3;q^3)_{n-3j-1}}\right). \tag{2.37}$$

Here, $\left[\begin{smallmatrix}a\\ b\end{smallmatrix}\right]_q$ is the q-binomial coefficient, defined by $\left[\begin{smallmatrix}a\\ b\end{smallmatrix}\right]_q = \frac{(q;q)_a}{(q;q)_{a-b}(q;q)_b}$ for integers $0 \leqslant b \leqslant a$, which is known to be a polynomial in q with non-negative coefficients.

We claim that the first factors in ((2.36)) and ((2.37)) are polynomials with non-negative coefficients if $j \leqslant (n-1)/6$. For $D_{n,j}(q)$, this is because the q-binomials and the polynomials

$$\frac{(q^3;q^3)_b(q;q)_a}{(q^3;q^3)_a(q;q)_b} = \prod_{k=a+1}^{b}(1+q^k+q^{2k})$$

have non-negative coefficients provided that $b \geqslant a$. In the case of $E_{n,j}(q)$, the factor

$$\frac{1-q^3}{1-q^{9j+3}}\begin{bmatrix}3j+1\\ j\end{bmatrix}_{q^3}$$

is the q-analogue of the Fuß–Catalan number (see, for example, Stump [Stu10]), and it is also a polynomial with non-negative coefficients.

On the other hand, if $(n-1)/3 > j > (n-1)/6$, then the first factors in ((2.36)) and ((2.37)) will no longer be polynomials. In these cases, we make the alternate factorizations

$$\begin{aligned} D_{n,j}(q) = {} & \left(q^{3j^2+3j}\begin{bmatrix}\lfloor (n-1)/3\rfloor + j + 1\\ 2j+1\end{bmatrix}_{q^3}\right) \\ & \times\left(\frac{(q^3;q^3)_{n-j-1}}{(q^3;q^3)_{\lfloor (n-1)/3\rfloor+j+1}}\frac{(q;q)_{3j+1}(q^3;q^3)_{\lfloor (n-1)/3\rfloor-j}}{(q^3;q^3)_j(q;q)_{n-3j-1}}\right), \end{aligned} \tag{2.38}$$

$$\begin{aligned} E_{n,j}(q) = {} & \left(q^{3j^2+3j}\begin{bmatrix}\lfloor (n-1)/3\rfloor + j + 1\\ 2j+1\end{bmatrix}_{q^3}\right) \\ & \times\left((1-q)\frac{(q^3;q^3)_{n-j-1}}{(q^3;q^3)_{\lfloor (n-1)/3\rfloor+j+1}}\frac{(q;q)_{3j}(q^3;q^3)_{\lfloor (n-1)/3\rfloor-j}}{(q^3;q^3)_j(q;q)_{n-3j-1}}\right), \end{aligned} \tag{2.39}$$

where the first factors in these equalities also has non-negative coefficients.

On the other hand, in each of the equalities ((2.36))–((2.39)), the second factor is a product of factors of the form $1-q^k$, with the single exception of the factor $(1+q^{3j+1}+q^{6j+2})/(1+q+q^2)$

(which is a polynomial) in ((2.37)). In order to certify the claim for ((2.38)) and ((2.39)), we note that

$$\frac{(q;q)_a(q^3;q^3)_{\lfloor b/3\rfloor}}{(q^3;q^3)_{\lfloor a/3\rfloor}(q;q)_b} = \prod_{\substack{k=b+1\\ 3\nmid k}}^{a}(1-q^k).$$

Therefore, the second factors in ((2.36))–((2.39)) are polynomials in q, possibly with some negative coefficients. To bound those polynomials from above, we note the trivial fact that $|1-q^k| \leqslant 1+|q|^k$, as well as the slightly non-trivial fact that

$$\begin{aligned}\left|\frac{1+q^{3j+1}+q^{6j+2}}{1+q+q^2}\right| &\leqslant \frac{|1-q^{6j+3}|+|q-q^{3j+1}|+|q^{3j+2}-q^{6j+2}|}{|1-q^3|}\\ &\leqslant \frac{1-|q|^{6j+3}}{1-|q|^3}+\frac{|q|-|q|^{3j+1}}{1-|q|^3}+\frac{|q|^{3j+2}-|q|^{6j+2}}{1-|q|^3}\\ &\leqslant \frac{1+|q|+|q|^2-|q|^{6j+1}-|q|^{6j+2}-|q|^{6j+3}}{1-|q|^3}\\ &= \frac{1-|q|^{6j+1}}{1-|q|},\end{aligned}$$

as long as $|q| \leqslant 1$ (where the $q=1$ case is understood in a limiting sense).

Based on these facts, we define the polynomials $\tilde{P}_{n,j}(r)$ for $P \in \{D,E\}$ to be the result of replacing q by r in the first parts of ((2.36))–((2.39)), replacing every factor $1-q^k$ in the second parts of ((2.36))–((2.39)) by a corresponding factor $1+r^k$, and replacing $(1+q^{3j+1}+q^{6j+2})/(1+q+q^2)$ in ((2.37)) by $(1-r^{6j+1})/(1-r)$. We also define $\tilde{F}_{n,j}(r) = r^{3j}\tilde{E}_{n,j}(r)$ in accordance with ((2.26)).

The immediate consequence of this definition are expressions for the quotients between successive $\tilde{P}_{n,j}(r)$'s. We have

$$\begin{aligned}\frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)} &= \frac{r^{3j-3/2}(1+r^{3n-9j})(1+r^{3n-9j+3})(1+r^{3n-9j+6})}{(1+r^{n-3j+1}+r^{2n-6j+2})(1+r^{n-3j+2}+r^{2n-6j+4})(1+r^{n-3j+3}+r^{2n-6j+6})(1+r^{3n-3j})}\\ &\quad\times\frac{r^{3j+3/2}(1-r^{3j-1})(1-r^{3j+1})}{(1-r^{6j+3})(1-r^{6j})} \quad \text{for } 1\leqslant j\leqslant \lfloor (n-1)/6\rfloor, \qquad (2.40)\\ \frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)} &= \frac{r^{3\lfloor(n-1)/3\rfloor-3/2}(1+r^{3j-1})(1+r^{3j+1})(1+r^{n-3j})(1+r^{n-3j+1})(1+r^{n-3j+2})}{(1+r^{3\lfloor(n-1)/3\rfloor+3j+3})(1+r^{3\lfloor(n-1)/3\rfloor-3j+3})(1+r^{3n-3j})}\\ &\quad\times\frac{r^{6j-3\lfloor(n-1)/3\rfloor+3/2}(1-r^{3\lfloor(n-1)/3\rfloor+3j})(1-r^{3\lfloor(n-1)/3\rfloor-3j})}{(1-r^{6j+3})(1-r^{6j})},\\ &\qquad\qquad \text{for } \lfloor(n-1)/6\rfloor+2\leqslant j\leqslant\lfloor(n-1)/3\rfloor, \qquad (2.41)\\ \frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)} &= \frac{\prod_{m=3j+\lfloor k/3\rfloor}^{3j+k-1}(1+r^{3m})\prod_{m=3j+k-5,3\nmid m}^{3j+1}(1+r^m)}{\prod_{m=3j-2}^{3j+k-2}(1+r^m+r^{2m})}\\ &\quad\times\frac{r^{6j}(1-r^{9j-3})\begin{cases}(1-r^{3j-3}) & k=0,1,2\\ (1-r^{9j}) & k=3,4,5\end{cases}}{(1-r^{6j+3})(1-r^{6j})},\end{aligned}$$

$$\text{for } j = \lfloor (n-1)/6 \rfloor + 1, \text{ or equivalently } n = 6(j-1) + k + 1 \text{ for } k = 0, 1, \ldots, 5. \tag{2.42}$$

for $\tilde{D}$, as well as

$$\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)} = \frac{r^{3j-3/2}(1+r^{3n-9j})(1+r^{3n-9j+3})(1+r^{3n-9j+6})}{(1+r^{n-3j+1}+r^{2n-6j+2})(1+r^{n-3j+2}+r^{2n-6j+4})(1+r^{n-3j+3}+r^{2n-6j+6})(1+r^{3n-3j})} \times \frac{r^{3j+3/2}(1-r^{3j-1})(1-r^{3j-2})(1-r^{6j+1})}{(1-r^{6j+3})(1-r^{6j})(1-r^{6j-5})} \text{ for } 1 \leqslant j \leqslant \lfloor (n-1)/6 \rfloor, \tag{2.43}$$

$$\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)} = \frac{r^{3\lfloor (n-1)/3 \rfloor}(1+r^{3j-1})(1+r^{3j-2})(1+r^{n-3j})(1+r^{n-3j+1})(1+r^{n-3j+2})}{(1+r^{3\lfloor (n-1)/3 \rfloor+3j+3})(1+r^{3\lfloor (n-1)/3 \rfloor-3j+3})(1+r^{3n-3j})} \times \frac{r^{6j-3\lfloor (n-1)/3 \rfloor}(1-r^{3\lfloor (n-1)/3 \rfloor+3j})(1-r^{3\lfloor (n-1)/3 \rfloor-3j})}{(1-r^{6j+3})(1-r^{6j})}, \quad \text{for } \lfloor (n-1)/6 \rfloor + 2 \leqslant j \leqslant \lfloor (n-1)/3 \rfloor, \tag{2.44}$$

$$\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)} = \frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)} \frac{(1+r)(1-r)(1-r^{9j-6})}{(1+r^{3j+1})(1-r^3)(1-r^{6j-3})}$$
$$\text{for } j = \lfloor (n-1)/6 \rfloor + 1, \text{ or equivalently } n = 6(j-1) + k + 1 \text{ for } k = 0, 1, \ldots, 5. \tag{2.45}$$

for $\tilde{E}$. Moreover, we trivially have

$$\frac{\tilde{F}_{n,j}(r)}{\tilde{F}_{n,j-1}(r)} = r^3 \frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)} \tag{2.46}$$

for all $j = 1, 2, \ldots, \lfloor (n-1)/3 \rfloor$. These relations will be used in the estimations of the tails and the remainders in Sections 2.10 and 2.11.

2.7 The cut-off values

In order to get a good balance among the error terms $\epsilon_{i,P}$, two cut-offs — θ_0 for the argument θ, and j_0 for the summation index j — will be chosen as

$$\theta_0 = \frac{1}{3} \frac{1-r}{1-r^n}, \tag{2.47}$$

$$j_0 = \lfloor \log_2 n \rfloor, \tag{2.48}$$

where r is the value of the saddle point given by the unique solution to ((2.33)).
Remark: One consequence of the choice ((2.47)) is that, whenever $q = re^{i\theta}$ with $0 < r \leqslant 1$ and $|\theta| < \theta_0$, we know that

$$k|\theta| < \frac{1}{3} \frac{k(1-r)}{(1-r^n)} \leqslant \frac{1}{3} \frac{(-\log(r^k))}{(1-r^k)}$$

for all k with $1 \leqslant k \leqslant n$. This means that the complex number q^k belongs to the region

$$\left\{ Re^{i\Theta} \,\middle|\, |\Theta| < \frac{1}{3}\frac{(-\log R)}{(1-R)} \right\}. \tag{2.49}$$

Having done all the preparatory work, we now dive into the estimations for the error terms $\epsilon_{i,P}$ in the next few sections.

2.8 Bounding the primary peak error

Lemma 2.8.1 *Suppose that r is chosen as the saddle point r_s defined in Lemma 2.5.1. Then, for all $n \geqslant 1500$, we have*

$$\epsilon_{0,P}(n,m,r) < \frac{7\sqrt{2}}{\sqrt{3\pi\lambda}} + \operatorname{erfc}\sqrt{\frac{\lambda}{84}},$$

where $\lambda = (r - r^{n+1})/(1-r)$. Here erfc *is the complementary Gaußian error function defined by* $\operatorname{erfc} x = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-x^2}dx$.

Proof: Note that the choice of r as the saddle point r_s of $P_{n,0}(re^{i\theta})e^{-im\theta}$ ensures that the Taylor expansion of $\log P_{n,0}(re^{i\theta})e^{-im\theta}$ at $\theta = 0$ has a vanishing linear term. Thus we can use Lemma 2.A.2 to bound the relative error $\epsilon_{0,P}(n,m,r_s)$. We define

$$h_{3,P}(n,r) = \sup_{|\theta|\leqslant\theta_0}\left|\frac{\partial^3}{\partial\theta^3}\log P_{n,0}(re^{i\theta})\right|,$$

Lemma 2.A.2 immediately allows us to conclude

$$\epsilon_{0,P}(n,m,r) \leqslant \operatorname{erfc}(\theta_0\sqrt{g_P(n,r)/2}) + 1.1 \times \frac{2\sqrt{2}}{3\sqrt{\pi}}\frac{h_{3,P}(n,r)}{g_P(n,r)^{3/2}}, \tag{2.50}$$

provided that $\theta_0 < (9g_P(n,r))/(4h_{3,P}(n,r))$.

The subsequent arguments in this part exploit some inequalities for the quantities $g_P(n,r)$, $h_{3,P}(n,r)$ and θ_0 to verify the conditions of Lemma 2.A.2.

We start by establishing simpler bounds on these three quantities. For the sake of simplicity, we write g and h for $g_P(n,r)$ and $h_{3,P}(n,r)$ in the subsequent arguments.

The definition of h implies that

$$h = h_{3,P}(n,r) \leqslant \sum_{k=1}^{n-1}\sup_{|\theta|\leqslant\theta_0}\left|\frac{ik^3q^k(1-q^{2k})(1+7q^k+q^{2k})}{(1+q^k+q^{2k})^3}\right|,$$

where $q = re^{i\theta}$. Therefore, an upper bound for h can be directly inferred from ((2.94)):

$$h \leqslant \frac{7}{5}\sum_{k=1}^{n} k^3r^k. \tag{2.51}$$

On the other hand, ((2.32)) and the elementary inequality $\frac{6}{5} > \frac{1+4r+r^2}{(1+r+r^2)^2} \geqslant \frac{2}{3}$ lead to the following bounds for g:

$$g < \frac{6}{5}\sum_{k=1}^{n} k^2 r^k, \tag{2.52}$$

as well as

$$\begin{aligned} g &\geqslant \frac{2}{3}\sum_{k=1}^{n} k^2 r^k - r - n^2 r^n \\ &\geqslant \left(\frac{2}{3} - \frac{n^2}{\sum_{k=1}^{n} k^2} - \left(\frac{1-r}{1-r^{n/2}}\right)^2\right)\sum_{k=1}^{n} k^2 r^k \\ &> \left(\frac{2}{3} - \frac{3}{n} - \frac{\alpha}{n}\right)\sum_{k=1}^{n} k^2 r^k \\ &> \left(\frac{2}{3} - \frac{1}{360}\right)\sum_{k=1}^{n} k^2 r^k, \end{aligned} \tag{2.53}$$

where we use the inequality $\sum_{k=1}^{n} k^2 r^k \geqslant \sum_{k=1}^{n} k^2 r^n$, as well as

$$\begin{aligned} \sum_{k=1}^{n} k^2 r^k \geqslant \sum_{k=1}^{n} k r^k &= \frac{r}{(1-r)^2}\left(1 + r^n - 2r^n\left(1 + \frac{n}{2}(1-r)\right)\right) \\ &\geqslant \frac{r}{(1-r)^2}\left(1 + r^n - 2r^n\left(1 + \frac{n}{2}(r^{-1}-1)\right)\right) \\ &\geqslant \frac{r}{(1-r)^2}\left(1 + r^n - 2r^n r^{-n/2}\right) = r\left(\frac{1-r^{n/2}}{1-r}\right)^2, \end{aligned}$$

and

$$n\left(\frac{1-r}{1-r^{n/2}}\right)^2 < n\left(\frac{1-\exp(-\sqrt{\alpha/n})}{1-\exp(-\sqrt{\alpha n}/2)}\right)^2 < \alpha,$$

which is a consequence of Lemma 2.5.1. We also need to recall from Lemma 2.5.1 that $\alpha = 2/\sqrt{3}$, so that the bound $n \geqslant 1500 > 120(9 + 2\sqrt{3})$ implies that $(3+\alpha)/n < 1/360$.

Having established the bounds above, we can establish some relationships among g, h, θ_0 and $\lambda = \sum_{k=1}^{n} r^k = \frac{r - r^{n+1}}{1-r}$.

The inequalities ((2.51)), ((2.53)) and ((2.98)) imply that

$$\begin{aligned} \theta_0 = \frac{r}{3\lambda} &\leqslant \frac{r}{3}\frac{(r^2+4r+1)}{r(r+1)}\frac{\sum_{k=1}^{n} k^2 r^k}{\sum_{k=1}^{n} k^3 r^k} \\ &\leqslant \frac{\sum_{k=1}^{n} k^2 r^k}{\sum_{k=1}^{n} k^3 r^k} < \frac{g/\left(\frac{2}{3} - \frac{1}{360}\right)}{5h/7} \\ &\leqslant \frac{45g/28}{5h/7} = \frac{9g}{4h}. \end{aligned}$$

We also infer from ((2.51)), ((2.53)) and ((2.99)) that

$$\begin{aligned}\frac{1.1\times 2\sqrt{2}}{3\sqrt{\pi}}\frac{h}{g^{3/2}} &< \frac{2\sqrt{2}}{3}\frac{\frac{7}{5}\times 1.1}{\sqrt{\pi}\left(\frac{2}{3}-\frac{4}{5n}\right)^{3/2}}\frac{\sum_{k=1}^{n}k^3r^k}{\left(\sum_{k=1}^{n}k^2r^k\right)^{3/2}}\\ &\leqslant \frac{2\sqrt{2}}{3}\frac{\frac{7}{5}\times 1.1}{\sqrt{\pi}\left(\frac{2}{3}-\frac{1}{360}\right)^{3/2}}\sqrt{\frac{(1+4r+r^2)^2}{(1+r)^3\sum_{k=1}^{n}r^k}} < \frac{2\sqrt{2}}{3}\frac{\frac{7}{5}\times\frac{10}{9}}{\sqrt{\pi}(\frac{2}{3})^{3/2}}\sqrt{\frac{9}{2\lambda}}\\ &= \frac{7\sqrt{2}}{\sqrt{3\pi\lambda}},\end{aligned}$$

where we used the numerical inequality $1.1\left(\frac{2}{3}-\frac{1}{360}\right)^{-3/2} < \frac{10}{9}\left(\frac{2}{3}\right)^{-3/2}$.

Finally, to bound the complementary error function in ((2.50)), which is equivalent to bound $g\theta_0^2$ from below, we invoke ((2.53)) and ((2.96)) to see that

$$g\theta_0^2 > \left(\frac{2}{3}-\frac{1}{360}\right)\frac{r}{3}\left(\frac{1-r^n}{1-r}\right)^3\left(\frac{1}{3}\frac{1-r}{1-r^n}\right)^2 > \frac{\lambda}{42},$$

and therefore

$$\operatorname{erfc}(\theta_0\sqrt{g/2}) > \operatorname{erfc}(\sqrt{\lambda/84}).$$

□

2.9 Bounding the secondary peaks

The error terms $\epsilon_{1,P}(n,r)$ related to the secondary peaks concern the quotients $\left|P_{n,j}(re^{i\theta})/P_{n,0}(re^{i\theta})\right|$. To bound these quotients from above, we look at the quotients of two consecutive polynomials.

$$\frac{D_{n,j}(q)}{D_{n,j-1}(q)} = \frac{q^{6j}(1-q^{n-3j})(1-q^{n-3j+1})(1-q^{n-3j+2})(1-q^{3j-1})(1-q^{3j+1})}{(1-q^{3n-3j})(1-q^{6j+3})(1-q^{6j})}, \tag{2.54}$$

$$\frac{E_{n,j}(q)}{E_{n,j-1}(q)} = \frac{q^{6j}(1-q^{n-3j})(1-q^{n-3j+1})(1-q^{n-3j+2})(1-q^{3j-1})(1-q^{3j-2})}{(1-q^{3n-3j})(1-q^{6j+3})(1-q^{6j})}. \tag{2.55}$$

Lemma 2.9.1 *Suppose that r_0 and θ_0 are as defined as in ((2.34)) and ((2.47)), respectively. Then, for all $j\in[1,\lfloor n/3\rfloor)$, all $q=re^{i\theta}\in\mathbb{C}$ such that $r\in(r_0,1]$, and $|\theta|<\theta_0$, we have*

$$\left|\frac{D_{n,j}(q)}{D_{n,j-1}(q)}\right| < (1.005+1.3/n)\frac{(3j+1)(3j-1)}{18j(2j+1)}\left(\frac{(j+1)\pi/n}{\sin((j+1)\pi/n)}\right)^2,$$

and

$$\left|\frac{E_{n,j}(q)}{E_{n,j-1}(q)}\right| < |q|^{-3/2}(1.005+1.3/n)\frac{(3j-1)(3j-2)}{18j(2j+1)}\left(\frac{(j+1)\pi/n}{\sin((j+1)\pi/n)}\right)^2.$$

Proof: We write $z = \frac{1}{2}\log q$ so that $e^{2z} = q$ and $(q^a - 1) = q^{a/2}\sinh az$. Note that the conditions on q imply the inequality

$$|\operatorname{Im} z| \leqslant \frac{1}{6}\frac{(1-e^{2\operatorname{Re} z})}{(1-e^{2n\operatorname{Re} z})}. \tag{2.56}$$

We claim that the inequality

$$\frac{1}{6}\frac{(1-e^{-2u})}{(1-e^{-2nu})} < \max\left(u, \frac{1}{3n}\right) < \sqrt{u^2 + \frac{1}{9n^2}} \tag{2.57}$$

holds for all $n \geqslant 1$ and all $u \geqslant 0$. This can be proved by observing that

$$\frac{1}{6}\frac{(1-e^{-2u})}{(1-e^{-2nu})} < \frac{u}{3}\frac{1}{(1-e^{-2nu})} < \frac{u}{3}\frac{1}{(1-e^{-1})} < u$$

if $u > \frac{1}{2n}$, and

$$\frac{1}{6}\frac{(1-e^{-2u})}{(1-e^{-2nu})} \leqslant \frac{1}{6}\frac{(1-e^{-1/n})}{(1-e^{-1})} < \frac{1}{6n}\frac{1}{(1-e^{-1})} < \frac{1}{3n}$$

if $u \leqslant \frac{1}{2n}$. Therefore, ((2.56)) and ((2.57)) imply that z satisfies the condition in Lemma 2.A.13 with $c = \frac{1}{3n} < \frac{\pi}{6n}$. Lemma 2.A.13 now says that, for any $a, b \in \mathbb{R}^+$ where $0 < a \leqslant b \leqslant 6n$, we have

$$\left|\frac{q^{(b-a)/2}(1-q^a)}{1-q^b}\right| \leqslant \frac{\sin(ac)}{\sin(bc)}. \tag{2.58}$$

We use ((2.58)) to bound various parts on the right-hand sides of ((2.54)) and ((2.55)). We have

$$\left|\frac{q^{3j-3}(1-q^{3n-9j+6})}{1-q^{3n-3j}}\right| \leqslant \frac{\sin\frac{n-3j+2}{2n}\pi}{\sin\frac{n-j}{2n}\pi} \leqslant 1,$$
$$\left|\frac{q^{3j-3/2}(1-q^{3n-9j+3})}{1-q^{3n-3j}}\right| \leqslant \frac{\sin\frac{n-3j+1}{2n}\pi}{\sin\frac{n-j}{2n}\pi} \leqslant 1,$$

as well as

$$\begin{aligned}\left|\frac{q^{(c+d-a-b)/2}(1-q^a)(1-q^b)}{(1-q^c)(1-q^d)}\right| &\leqslant \frac{\sin\frac{a}{6n}\pi\,\sin\frac{b}{6n}\pi}{\sin\frac{c}{6n}\pi\,\sin\frac{d}{6n}\pi} \\ &< \frac{ab}{cd}\left(\frac{c\pi/6n}{\sin(c\pi/6n)}\frac{d\pi/6n}{\sin(d\pi/6n)}\right) < \frac{ab}{cd}\left(\frac{(j+1)\pi/n}{\sin((j+1)\pi/n)}\right)^2,\end{aligned}$$

for $(a,b,c,d) = (3j-1, 3j+1, 6j+3, 6j)$ or $(3j-1, 3j-2, 6j+3, 6j)$.

It remains to bound the factor

$$\left|\frac{(1-q^{k-1})(1-q^{k+1})}{1+q^k+q^{2k}}\right|,$$

where $k = n - 3j + 1$ or $n - 3j + 2$. Here we make use of ((2.92)) and ((2.93)) (recall that q^k belongs to the region ((2.49))) to conclude that

$$\begin{aligned}\left|\frac{(1-q^{k-1})(1-q^{k+1})}{1+q^k+q^{2k}}\right| &\leqslant \left|\frac{(1-q^k)^2}{1+q^k+q^{2k}}\right| + \left|\frac{q^{k-1}(1-q)^2}{1+q^k+q^{2k}}\right| \\ &< 1.005 + 1.002|1-q|^2 \\ &< 1.005 + 1.002((1-r)^2+\theta_0^2)) \\ &\leqslant 1.005 + 1.002\left(\frac{2}{\sqrt{3}n}(1+\frac{1}{9})\right) \\ &< 1.005 + 1.3/n. \end{aligned}$$

□

These bounds allow us to obtain upper bounds for the first factor in the expression ((2.16)) of the error term $\epsilon_{1,P}(n,r)$.

Lemma 2.9.2 *Suppose $n > 7000$, and that r_0, j_0 and θ_0 are defined as in ((2.34)), ((2.48)) and ((2.47)), respectively. Then, for all $r \in (r_0, 1]$, we have*

$$\sum_{j=1}^{j_0} \sup_{|\theta|<\theta_0} \left|\frac{D_{n,j}\left(re^{i\theta}\right)}{D_{n,0}\left(re^{i\theta}\right)}\right| < 0.187,$$

$$\sum_{j=1}^{j_0} \sup_{|\theta|<\theta_0} \left|\frac{E_{n,j}\left(re^{i\theta}\right)}{E_{n,0}\left(re^{i\theta}\right)}\right| < 0.043,$$

$$\sum_{j=1}^{j_0} \sup_{|\theta|<\theta_0} \left|\frac{F_{n,j}\left(re^{i\theta}\right)}{F_{n,0}\left(re^{i\theta}\right)}\right| < 0.043.$$

Proof: We first make use of Lemma 2.9.1, and we notice that the condition $n > 7000$ and the choice of j_0 imply that $(j+1)/n < \frac{\log n + \log 2}{n \log 2} < \frac{1}{500}$. Therefore, the terms involving n in Lemma 2.9.1 can be bounded above by

$$(1.005 + 1.3/7000)\left(\frac{\pi/500}{\sin \pi/500}\right)^2 < 1.006.$$

This implies

$$\left|\frac{D_{n,j}(q)}{D_{n,0}(q)}\right| < 1.006^j \prod_{k=1}^{j} \frac{(3k+1)(3k-1)}{18k(2k+1)} = \frac{1.006^j}{27^j}\binom{3j+1}{j},$$

and

$$\left|\frac{E_{n,j}(q)}{E_{n,0}(q)}\right| < 1.006^j \prod_{k=1}^{j} |q|^{-3k/2} \frac{(3k-1)(3k-2)}{18k(2k+1)} = \frac{(1.006|q|^{-3/2})^j}{27^j(3j+1)}\binom{3j+1}{j},$$

for all j with $1 \leqslant j \leqslant j_0$. The relationship ((2.26)) implies a similar inequality for $F_{n,j}$, namely

$$\left|\frac{F_{n,j}(q)}{F_{n,0}(q)}\right| < 1.006^j \prod_{k=1}^{j} |q|^{3k/2} \frac{(3k-1)(3k-2)}{18k(2k+1)} = \frac{(1.006|q|^{3/2})^j}{27^j(3j+1)} \binom{3j+1}{j}.$$

The bounds stated in the lemma can be obtained by noticing that

$$|q|^{-3/2} \leqslant r_0^{-3/2} = \exp\left(\sqrt{\sqrt{3}/n}\right) < \exp\left(\sqrt{\sqrt{3}/7000}\right) < 1.0003,$$

and by using the identities (cf. [PBM90, Section 7.3.2])

$$\sum_{j=0}^{\infty} \frac{a^j}{27^j} \binom{3j+1}{j} = \frac{6}{\sqrt{4a-a^2}} \sin\left(\frac{2}{3}\sin^{-1}\frac{\sqrt{a}}{2}\right),$$

$$\sum_{j=0}^{\infty} \frac{a^j}{(3j+1)27^j} \binom{3j+1}{j} = \frac{6}{\sqrt{a}} \sin\left(\frac{1}{3}\sin^{-1}\frac{\sqrt{a}}{2}\right),$$

to give the estimates

$$\sum_{j=1}^{\infty} \frac{1.006^j}{27^j} \binom{3j+1}{j} \approx 0.18618 < 0.187,$$

$$\sum_{j=1}^{\infty} \frac{(1.006 \times 1.0003)^j}{27^j(3j+1)} \binom{3j+1}{j} \approx 0.04219 < 0.043,$$

$$\sum_{j=1}^{\infty} \frac{1.006^j}{27^j(3j+1)} \binom{3j+1}{j} \approx 0.04218 < 0.043. \qquad \square$$

Here and in the subsequent parts of the paper, the $\approx$ symbol signifies that the approximation value given is accurate to the last significant figure.

It remains to deal with the second factor in ((2.16)), namely

$$\sqrt{\frac{g_P(n,r)}{2\pi}} \int_{-\theta_0}^{\theta_0} \left|\frac{P_{n,0}(re^{i\theta})}{P_{n,0}(r)}\right| d\theta.$$

The argument below is parallel to the one in Section 2.8.

Lemma 2.9.3 *Suppose that $n \geqslant 1500 > 120(9+2\sqrt{3})$, and θ_0 is defined as in ((2.47)). Then we have*

$$\sqrt{\frac{g_P(n,r)}{2\pi}} \int_{-\theta_0}^{\theta_0} \left|\frac{P_{n,0}(re^{i\theta})}{P_{n,0}(r)}\right| d\theta \leqslant 1 + \frac{\sqrt{5}}{3\sqrt{3\lambda}},$$

where $\lambda = \frac{r-r^{n+1}}{1-r}$.

Proof: Note that the integrand is an even function in θ, so we can use Lemma 2.A.4 to bound the integral. We define

$$h_{4,P}(n,r) = \sup_{|\theta| \leqslant \theta_0} \left|\frac{\partial^4}{\partial\theta^4} \log P_{n,0}(re^{i\theta})\right|,$$

Lemma 2.A.2 immediately allows us to conclude

$$\sqrt{\frac{g_P(n,r)}{2\pi}}\int_{-\theta_0}^{\theta_0}\left|\frac{P_{n,0}(re^{i\theta})}{P_{n,0}(r)}\right|d\theta \leqslant 1+\frac{\sqrt{2}}{9\sqrt{\pi}}\frac{h_{4,P}(n,r)^{1/2}}{g_P(n,r)}, \tag{2.59}$$

provided that the condition $\theta_0^2 < (27g_P(n,r))/(8h_{4,P}(n,r))$ is satisfied.

The subsequent arguments in this part exploit some inequalities for the quantities $g_P(n,r)$, $h_{4,P}(n,r)$ and θ_0 to verify the conditions of Lemma 2.A.4.

We start by establishing simpler bounds on them. For the sake of simplicity, we write g and h for $g_P(n,r)$ and $h_{4,P}(n,r)$ in the subsequent arguments.

The definition of h implies that

$$h = h_{4,P}(n,r) \leqslant \sum_{k=1}^{n-1}\sup_{|\theta|\leqslant\theta_0}\left|\frac{k^4q^k(1+12q^k-12q^{2k}-56q^{3k}-12q^{4k}+12q^{5k}+q^{6k})}{(1+q^k+q^{2k})^4}\right|,$$

where $q = re^{i\theta}$.

Therefore, an upper bound for h can be directly inferred from ((2.95)):

$$h < \frac{5}{3}\sum_{k=1}^{n}k^4r^k. \tag{2.60}$$

On the other hand, we recall the upper and lower bounds on g from ((2.52)) and ((2.53)). We establish some relationships among g, h, θ_0 and $\lambda = \sum_{k=1}^{n} r^k = \frac{r-r^{n+1}}{1-r}$.

The inequalities ((2.60)), ((2.53)) and ((2.100)) imply that

$$\begin{aligned}\theta_0^2 = \frac{r^2}{9\lambda^2} &\leqslant \frac{r^2}{9}\frac{1+10r+r^2}{r^2}\frac{\sum_{k=1}^{n}k^2r^k}{\sum_{k=1}^{n}k^4r^k}\\ &\leqslant \frac{4}{3}\frac{\sum_{k=1}^{n}k^2r^k}{\sum_{k=1}^{n}k^3r^k} < \frac{4}{3}\frac{g/\left(\frac{2}{3}-\frac{1}{360}\right)}{3h/5}\\ &\leqslant \frac{27g}{8h}.\end{aligned}$$

Moreover, from ((2.60)), ((2.53)) and ((2.101)), we also infer that

$$\begin{aligned}\frac{\sqrt{2}}{9\sqrt{\pi}}\frac{h^{1/2}}{g} &< \frac{\sqrt{2}}{9\sqrt{\pi}}\frac{\sqrt{5/3}}{\frac{2}{3}-\frac{1}{360}}\frac{\left(\sum_{k=1}^{n}k^4r^k\right)^{1/2}}{\sum_{k=1}^{n}k^2r^k}\\ &\leqslant \frac{\sqrt{2}}{9\sqrt{3}}\frac{\sqrt{5/3}}{2/3}\sqrt{\frac{1+10r+r^2}{(1+r)\left(\sum_{k=1}^{n}r^k\right)}} \leqslant \frac{\sqrt{5}}{9\sqrt{2}}\sqrt{\frac{6}{\lambda}}\\ &= \frac{\sqrt{5}}{3\sqrt{3\lambda}}.\end{aligned}$$

□

By combining Lemmas 2.9.2 and 2.9.3, we arrive at our bound for the error term $\epsilon_{1,P}(n,r)$.

Lemma 2.9.4 *For all $n > 7000$ and all r with $0 < r \leqslant 1$, we have*

$$\epsilon_{1,D}(n,r) < 0.187\left(1+\frac{\sqrt{5}}{3\sqrt{3\lambda}}\right),$$
$$\epsilon_{1,E}(n,r) < 0.043\left(1+\frac{\sqrt{5}}{3\sqrt{3\lambda}}\right),$$
$$\epsilon_{1,F}(n,r) < 0.043\left(1+\frac{\sqrt{5}}{3\sqrt{3\lambda}}\right).$$

2.10 Bounding the remainders

The reason we estimate the remainder parts before the tail is that certain results in this section, namely upper bounds for the ratios $\left|\tilde{P}_{n,j}(r)/\tilde{P}_{n,j-1}(r)\right|$, will also be used in bounding the tails from above.

Lemma 2.10.1 *Suppose that $n \in \mathbb{Z}^+$, and $0 < r \leqslant 1$. For all $j \in [1, \lfloor (n-1)/6 \rfloor]$, we have*

$$\left|\frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)}\right| < \frac{(3j-1)(3j+1)}{18j(2j+1)}, \qquad \left|\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)}\right| < \frac{r^{-3/2}(3j-1)(3j-2)(6j+1)}{18j(2j+1)(6j-5)}.$$

For all $j \in [\lfloor (n-1)/6 \rfloor + 2, \lfloor (n-1)/3 \rfloor]$, we have

$$\left|\frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)}\right| < \frac{4(\lfloor (n-1)/3 \rfloor - j)}{3j - \lfloor (n-1)/3 \rfloor + 1}, \qquad \left|\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)}\right| < \frac{4r^{-3/2}(\lfloor (n-1)/3 \rfloor - j)}{(3j - \lfloor (n-1)/3 \rfloor + 1)}.$$

Finally for $j = \lfloor (n-1)/6 \rfloor + 1$ we have

$$\left|\frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,j-1}(r)}\right| < 72, \qquad \left|\frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,j-1}(r)}\right| < 72.$$

Proof: We claim that the first factors in ((2.40)) and ((2.43)) do not exceed 1, and the first factors in ((2.41)) and ((2.44)) do not exceed 4. The claims about ((2.40)) and ((2.43)) are proved by using the inequality $1 + r^{3k} < 1 + r^{k+1} + r^{2k+2}$ for $k = n-3j, n-3j+1, n-3j+2$, and the claims about ((2.41)) and ((2.44)) are proved by observing that

$$\frac{(1+r^{n-3j})(1+r^{n-3j+1})(1+r^{n-3j+2})}{(1+r^{3\lfloor (n-1)/3 \rfloor - 3j+3})} \leqslant 4,$$

as well as the inequality $r^{(b-a)/2}(1+r^a) \leqslant 1 + r^b$, valid for $0 < r < 1$ and $0 < a < b$.

The second factors in ((2.40)) and ((2.43)) can be estimated using the inequality $r^{(b-a)/2}(1-r^a)/(1-r^b) \leqslant a/b$, valid for all $r \in \mathbb{R}$ and $b \geqslant a > 0$. (This can be considered as a limiting form of Lemma 2.A.13 when $c \to 0$.) In order to deal with the factor $(1-r^{6j+1})/(1-r^{6j-5})$, we use the fact that the function $a \mapsto (1-r^a)/a$ is decreasing in a if $0 < r \leqslant 1$. This concludes the proof of the first part of the lemma.

We cannot directly use the same method for the second factors in ((2.41)) and ((2.44)) because, in each case, one exponent in the numerator, namely $3\lfloor (n-1)/3 \rfloor + 3j$, would be larger than both exponents in the denominator. Instead, we argue that if $a \geqslant c \geqslant d \geqslant b$ and $c + d \geqslant a + b$,

then we have

$$\frac{r^{(c+d-a-b)/2}(1-r^a)(1-r^b)}{(1-r^c)(1-r^d)} \leqslant \frac{b}{c+d-a}\frac{(1-r^a)(1-r^{c+d-a})}{(1-r^c)(1-r^d)} \leqslant \frac{b}{c+d-a}.$$

Insertion of specific values of a, b, c, d from ((2.41)) and ((2.44)) into the above inequality concludes the proof for the first four cases. For the borderline cases where $j = \lfloor (n-1)/6 \rfloor + 1$, we note the following facts:

- The numerator of the first factor in ((2.42)) consists of exactly 5 factors of the form $1 + r^m$, so the first factor can be bounded above by 2^5;
- The second factor in ((2.42)) can be bounded above by $9/4$;
- Finally, the extra factor in ((2.45)) can be bounded above by 1.

Combining the three ovservations concludes the proof for the borderline cases. □

Lemma 2.10.2 *Suppose that $n > 7000$, and that r_0, j_0 and θ_0 are as defined as in ((2.34)), ((2.48)) and ((2.47)), respectively. Then, for all $r \in (r_0, 1]$, we have*

$$\epsilon_{3,D}(n,r) < 0.004, \qquad \epsilon_{3,E}(n,r) < 0.008, \qquad \epsilon_{3,F}(n,r) < 0.008.$$

Proof: Lemma 2.10.1 implies the following inequalities for $\tilde{D}_{n,j}$ and $\tilde{E}_{n,j}$:

$$\frac{\tilde{D}_{n,j}(r)}{D_{n,0}(r)} \leqslant \binom{3j+1}{j} 3^{-3j}, \qquad \text{for } 0 \leqslant j \leqslant \lfloor (n-1)/6 \rfloor, \tag{2.61}$$

$$\frac{\tilde{D}_{n,j}(r)}{D_{n,\lfloor (n-1)/6+1 \rfloor}(r)} \leqslant \prod_{k=\lfloor (n-1)/6 \rfloor+2}^{j} \frac{4(\lfloor (n-1)/3 \rfloor - k + 1)}{(3k - \lfloor (n-1)/3 \rfloor - 1)}, \quad \text{for } \lfloor (n-1)/6 \rfloor < j \leqslant \lfloor (n-1)/3 \rfloor, \tag{2.62}$$

$$\frac{\tilde{E}_{n,j}(r)}{E_{n,0}(r)} \leqslant \frac{6j+1}{3j+1} r^{-3j/2} \binom{3j+1}{j} 3^{-3j}, \qquad \text{for } 0 \leqslant j \leqslant \lfloor (n-1)/6 \rfloor, \tag{2.63}$$

$$\frac{\tilde{E}_{n,j}(r)}{E_{n,\lfloor (n-1)/6+1 \rfloor}(r)} \leqslant \prod_{k=\lfloor (n-1)/6 \rfloor+2}^{j} \frac{4(\lfloor (n-1)/3 \rfloor - k + 1)}{(3k - \lfloor (n-1)/3 \rfloor - 1)}, \quad \text{for } \lfloor (n-1)/6 \rfloor < j \leqslant \lfloor (n-1)/3 \rfloor. \tag{2.64}$$

From Lemma 2.10.1, we can also provide bounds for the borderline case:

$$\frac{\tilde{D}_{n,\lfloor (n-1)/6+1 \rfloor}(r)}{D_{n,\lfloor (n-1)/6 \rfloor}(r)} \leqslant 72, \qquad \frac{\tilde{E}_{n,\lfloor (n-1)/6+1 \rfloor}(r)}{E_{n,\lfloor (n-1)/6 \rfloor}(r)} \leqslant 72.$$

We observe that the factor $\frac{4(K-k+1)}{(3k-K-1)}$ does not exceed 4 for all $k \in [(K+1)/2, K]$, and it does not exceed 1 for all $k \in [5(K+1)/7, K]$. Therefore, the right-hand sides of ((2.62)) and ((2.64)) (where $K = \lfloor (n-1)/3 \rfloor$) can be bounded above by

$$4^{(\frac{5}{7}-\frac{1}{2})(K+1)} \leqslant 4^{\frac{3}{14}(\lfloor n/3 \rfloor+1)} < 2^{n/7+1}.$$

Taking into account the inequality $\binom{3j+1}{j}3^{-3j} < 4^{-j}\sqrt{\frac{27}{16\pi j}}$, we compute

$$\begin{aligned}\sum_{j=j_0+1}^{\lfloor (n-1)/3 \rfloor} \frac{\tilde{D}_{n,j}(r)}{D_{n,0}(r)} &< \sum_{j=j_0+1}^{\infty} 4^{-j}\sqrt{\frac{27}{16\pi j}} + 72(n/6)4^{-n/6}\sqrt{\frac{27}{16\pi n/6}}2^{n/7+1} \\ &\leqslant 4^{-j_0}\sqrt{\frac{3}{\pi j_0}} + \sqrt{\frac{n}{\pi}}2^{n/7-n/3+3/2}3^3 \\ &\leqslant n^{-2}\sqrt{\frac{4\log 2}{2\pi \log n}} + 2^{3/2-4n/21}3^3\sqrt{\frac{n}{\pi}}.\end{aligned}$$

Applying analogous arguments, and by using the inequality $\frac{6j+1}{3j+1} < 2$, we get

$$\sum_{j=j_0+1}^{\lfloor (n-1)/3 \rfloor} \frac{\tilde{E}_{n,j}(r)}{E_{n,0}(r)} < n^{-2}\sqrt{\frac{12\log 2}{\pi \log n}} + 2^{5/2-4n/21}3^3\sqrt{\frac{n}{\pi}}.$$

Finally, using the fact that

$$g_P(n,r) \leqslant g_P(n,1) = \sum_{k=2}^{n-1} \frac{2}{3}k^2 = \frac{2n^3-3n^2+n-6}{9} < \frac{2}{9}n^3$$

for $n \geqslant 2$, we conclude that

$$\varepsilon_{3,D}(n,r) \leqslant \sqrt{\frac{4\log 2}{3n\log n}} + 2^{5/2-4n/21}3^2n^2,$$

and

$$\varepsilon_{3,E}(n,r) \leqslant \sqrt{\frac{16\log 2}{3n\log n}} + 2^{7/2-4n/21}3^2n^2.$$

We finish the proof by using the condition $n > 7000$ in the above bounds, and by recalling ((2.46)) to draw a similar conclusion about $\varepsilon_{3,F}(n,r)$. □

2.11 Bounding the tails

In order to bound the error term $\epsilon_{2,P}(n,r)$, we need bounds on $P_{n,j}(re^{i\theta})/\tilde{P}_{n,j}(r)$ as well as on $\tilde{P}_{n,j}(r)/\tilde{P}_{n,0}(r)$. The results of previous section, along with ((2.46)), imply the inequalities

$$\sum_{j=0}^{j_0} \frac{\tilde{D}_{n,j}(r)}{\tilde{D}_{n,0}(r)} < \sum_{j=0}^{\infty} 3^{-3j} \binom{3j+1}{j} < 1.185, \tag{2.65}$$

$$\sum_{j=0}^{j_0} \frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,0}(r)} < \sum_{j=0}^{\infty} 3^{-3j} \binom{3j+1}{j} 1.003^j \frac{6j+1}{3j+1} < 1.329, \tag{2.66}$$

$$\sum_{j=0}^{j_0} \frac{\tilde{F}_{n,j}(r)}{\tilde{F}_{n,0}(r)} < \sum_{j=0}^{j_0} \frac{\tilde{E}_{n,j}(r)}{\tilde{E}_{n,0}(r)} < 1.329. \tag{2.67}$$

We now turn our attention to the quotient $P_{n,j}(re^{i\theta})/\tilde{P}_{n,j}(r)$.

Proposition 2.11.1 *For all $n > 32$, $r \in (0,1]$, $\theta \in [-\pi,\pi]$ and $0 \leqslant j \leqslant j_0$, we have*

$$\left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| < \exp\left(-\phi(n, 3j_0+2, n-6j_0-2, r, \rho)\right),$$

where $\rho = \theta\frac{1-r^n}{1-r}$, and

$$\phi(n,a,b,r,\rho) := \frac{b^3}{n^3}\frac{r^a}{1+r^{2a}}\frac{(1+r)^2}{4}\frac{1-r^{n/12}}{1-r}\left(1-\sqrt{\frac{1+\frac{(1-r)^2(1+r^b)^2}{(1+r)^2(1-r^b)^2}\rho^2}{1+\rho^2}}\right).$$

Proof: The condition $n > 32$ ensures that $n > 6j_0+2$. Therefore, Lemma 2.A.5 implies that

$$\begin{aligned}
-\log\left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| &\geqslant \sum_{m=3j+2}^{n-3j-1} -\log\left|\frac{1+r^m e^{im\theta}+r^{2m}e^{2im\theta}}{1+r^m+r^{2m}}\right| \\
&\geqslant \sum_{m=3j_0+2}^{n-3j_0-1} \frac{2r^m}{1+r^{2m}}\sin(m\theta/2)^2 \\
&\geqslant \frac{2r^a}{1+r^{2a}}\sum_{m=a}^{a+b-1} r^{m-a}\sin(m\theta/2)^2,
\end{aligned}$$

where we write $a = 3j_0+2$ and $b = n-6j_0-2$ for simplicity of notation.

Now Lemma 2.A.8 allows us to do further estimation:

$$-\log\left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| \geqslant \frac{r^a}{1+r^{2a}}\frac{1-r^b}{1-r}\left(1-\sqrt{\frac{1+\kappa\frac{(1+r^b)^2}{(1-r^b)^2}\tan^2(\theta/2)}{1+\kappa\frac{(1+r)^2}{(1-r)^2}\tan^2(\theta/2)}}\right),$$

where

$$\kappa = \frac{(1-r^b)(1-r^{b/3})}{(1+r^b)(1+r^{b/3})}.$$

After substituting $\theta = \rho\frac{1-r}{1-r^n}$, we first note

$$\tan\frac{\theta}{2} \geqslant \frac{\theta}{2} = \frac{\rho}{2}\frac{1-r}{1-r^n},$$

valid for $|\theta| \leqslant \pi$. Then we use the fact that $\frac{1+cx}{1+cy}$ is decreasing with respect to c if $y > x > 0$ to estimate the factor in terms of ρ:

$$1 - \sqrt{\frac{1+\kappa\frac{(1+r^b)^2}{(1-r^b)^2}\tan^2(\theta/2)}{1+\kappa\frac{(1+r)^2}{(1-r)^2}\tan^2(\theta/2)}} \geqslant 1 - \sqrt{\frac{1+\kappa\frac{(1+r^b)^2(1-r)^2}{4(1-r^b)^2(1-r^n)^2}\rho^2}{1+\kappa\frac{(1+r)^2}{4(1-r^n)^2}\rho^2}}.$$

By exploiting the inequality

$$1 - \sqrt{\frac{1+cx}{1+cy}} \geqslant c\left(1 - \sqrt{\frac{1+x}{1+y}}\right)$$

for all $0 < c \leqslant 1$ and $y > x > 0$, and by taking

$$c = \kappa\frac{(1+r)^2}{4(1-r^n)^2} = \frac{(1+r)^2}{4}\frac{1-r^{b/3}}{1-r^b}\left(\frac{1-r^b}{1-r^n}\right)^2\frac{1}{(1+r^b)(1+r^{b/3})} \leqslant 1,$$

we arrive at the expected result:

$$\begin{aligned}
-\log\left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| &\geqslant \frac{r^a}{1+r^{2a}}\frac{1-r^{b/3}}{1-r}\left(\frac{1-r^b}{1-r^n}\right)^2\frac{(1+r)^2}{4(1+r^b)(1+r^{b/3})}\left(1-\sqrt{\frac{1+\frac{(1-r)^2(1+r^b)^2}{(1+r)^2(1-r^b)^2}\rho^2}{1+\rho^2}}\right)\\
&= \frac{r^a}{1+r^{2a}}\frac{1-r^{b/12}}{1-r}\left(\frac{1-r^b}{1-r^n}\right)^2\frac{(1+r)^2(1+r^{b/6})(1+r^{b/12})}{4(1+r^b)(1+r^{b/3})}\\
&\qquad\times\left(1-\sqrt{\frac{1+\frac{(1-r)^2(1+r^b)^2}{(1+r)^2(1-r^b)^2}\rho^2}{1+\rho^2}}\right)\\
&\geqslant \frac{b^3}{n^3}\frac{r^a}{1+r^{2a}}\frac{1-r^{n/12}}{1-r}\frac{(1+r)^2}{4}\left(1-\sqrt{\frac{1+\frac{(1-r)^2(1+r^b)^2}{(1+r)^2(1-r^b)^2}\rho^2}{1+\rho^2}}\right),
\end{aligned}$$

where the last step uses the inequality $\frac{1-r^x}{1-r^y} > \frac{x}{y}$, valid for $0 \leqslant r \leqslant 1$ and $y \geqslant x$. □

In order to convert the above lemma into an upper bound for $\epsilon_{2,P}(n,r)$, we first note that $\phi(n,a,b,r,\rho)$ is increasing with respect to ρ. We estimate the integral in the definition of $\epsilon_{2,P}(n,r)$ by making the substitution $\theta = \frac{1-r}{1-r^n}\rho$ as in Proposition 2.11.1 and by splitting the

integral at $\rho = \frac{3}{2}$, as shown below:

$$\begin{aligned}\int_{\theta_0}^{2\pi-\theta_0} \sup_{0\leqslant j\leqslant j_0} \left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| d\theta &\leqslant 2\frac{1-r}{1-r^n}\int_{1/3}^{\pi\frac{1-r^n}{1-r}} \exp\left(-\phi(n,3j_0+2,n-6j_0-2,r,\rho)\right) d\rho \\ &\leqslant 2\frac{1-r}{1-r^n}\left(\int_{1/3}^{3/2}+\int_{3/2}^{\pi\frac{1-r^n}{1-r}}\right)\exp\left(-\phi(n,3j_0+2,n-6j_0-2,r,\rho)\right) d\rho \\ &< 2\frac{1-r}{1-r^n}\int_{1/3}^{3/2}\exp\left(-\phi(n,3j_0+1,n-6j_0,r,\rho)\right) d\rho \\ &\qquad + 2\pi\exp\left(-\phi(n,3j_0+2,n-6j_0-2,r,3/2)\right).\end{aligned}$$

Suppose for now that $n > 7000$ and $r \in (r_0, 1]$. By looking at the various factors in the definition of $\phi(n,a,b,r,\rho)$, we observe that

$$\begin{aligned}\frac{n-6j_0-2}{n} &\geqslant 1-\frac{6\log_2 n+2}{n} > 0.9887, \\ r^{3j_0+2} &\geqslant \exp\left(-(3\log_2 n+2)\sqrt{\alpha/n}\right) > 0.5958, \\ \frac{(1+r)^2}{4} &\geqslant \frac{(1+r_0)^2}{4} > \frac{74}{75}, \\ \frac{(1-r)(1+r^b)}{(1+r)(1-r^b)} &\leqslant \frac{(1-r_0)(1+r_0^n)}{(1+r_0)(1-r_0^n)} < \frac{1}{150}.\end{aligned}$$

These observations enable us to conclude

$$\begin{aligned}\phi(n,3j_0+2,n-6j_0-2,r,\rho) &> 0.9887^3\frac{0.5958}{1+(0.5958)^2}\frac{74}{75}\left(1-\sqrt{\frac{1+(\rho/150)^2}{1+\rho^2}}\right)\frac{1-r^{n/12}}{1-r} \\ &> \frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+\rho^2}}\right)\frac{1-r^{n/12}}{1-r},\end{aligned}$$

for all $n > 7000$ and $\rho \in [1/3, 3/2]$. We define

$$\phi^*(n,r,\rho) := \frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+\rho^2}}\right)\frac{1-r^{n/12}}{1-r}, \tag{2.68}$$

and obtain that

$$\begin{aligned}&\int_{\theta_0}^{2\pi-\theta_0} \sup_{0\leqslant j\leqslant j_0} \left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| d\theta \\ &\quad < 2\frac{1-r}{1-r^n}\int_{1/3}^{3/2}\exp\left(-\phi(n,3j_0+1,n-6j_0,r,\rho)\right) d\rho \\ &\qquad + 2\pi\exp\left(-\phi(n,3j_0+2,n-6j_0-2,r,3/2)\right) \\ &\quad < 2\frac{1-r}{1-r^n}\int_{1/3}^{3/2}\exp\left(-\phi^*(n,r,\rho)\right) d\rho + 2\pi\exp\left(-\phi^*(n,r,3/2)\right).\end{aligned} \tag{2.69}$$

At this point, we incorporate the factor $\sqrt{g_P(n,r)}$ in the definition of $\epsilon_{2,P}(n,r)$. We note that, using ((2.52)) and ((2.97)), we have

$$g_P(n,r) < \frac{12}{5}\left(\frac{1-r^n}{1-r}\right)^3. \tag{2.70}$$

In view of this upper bound, we prove some related monotonicity results.

Lemma 2.11.2 *Let ϕ^* be defined as in ((2.68)). For all $n > 7000$ and all $r \in (r_0, 1]$, we have:*

- *The function*

$$\left(\frac{1-r^n}{1-r}\right)^{3/2} \exp\left(-\phi^*(n,r,3/2)\right) \tag{2.71}$$

  is decreasing with respect to r.

- *If $\rho \in [1/3, 3/2]$, then the function*

$$\left(\frac{1-r^n}{1-r}\right)^{1/2} \exp\left(-\phi^*(n,r,\rho)\right) \tag{2.72}$$

  is also decreasing with respect to r.

Proof: By taking logarithmic derivatives with respect to r, these claims are equivalent to the inequalities

$$\frac{3}{2}\frac{\partial}{\partial r}\log\frac{1-r^n}{1-r} \leqslant \frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+(3/2)^2}}\right)\frac{\partial}{\partial r}\frac{1-r^{n/12}}{1-r}, \tag{2.73}$$

and

$$\frac{1}{2}\frac{\partial}{\partial r}\log\frac{1-r^n}{1-r} \leqslant \frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+\rho^2}}\right)\frac{\partial}{\partial r}\frac{1-r^{n/12}}{1-r}. \tag{2.74}$$

In order to prove ((2.73)) and ((2.74)), we perform the following calculations:

- Lemmas 2.A.11 and 2.A.12 imply that

$$\frac{\partial}{\partial r}\frac{1-r^{n/12}}{1-r} \geqslant \frac{(1-r^{n/12})(1-r^{(n-12)/24})}{(1-r)^2} \geqslant 24\frac{1-r^n}{1-r}.$$

- Again, Lemma 2.A.11 imply that

$$\frac{\partial}{\partial r}\log\frac{1-r^n}{1-r} \leqslant \frac{1-r^n}{1-r}.$$

- We have [2]

$$\frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+(3/2)^2}}\right) \approx 0.18553 > \frac{1}{6},$$

  therefore the right-hand side of ((2.73)) is at least $4\frac{1-r^n}{1-r}$.

[2] The reader is referred to the remark after Lemma 2.9.2 for the meaning of the symbol $\approx$.

- Since $\rho \geqslant 1/3$, we have

$$\frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+\rho^2}}\right) \geqslant \frac{5}{12}\left(1-\sqrt{\frac{1+10^{-4}}{1+1/9}}\right) \approx 0.021362 > \frac{1}{48},$$

□

and thus the right-hand side of ((2.74)) is at least $\frac{1}{2}\frac{1-r^n}{1-r}$. □

We are now ready to provide explicit upper bounds for $\epsilon_{2,P}(n,r)$.

Lemma 2.11.3 *Suppose that $n > n_0 = 7000$, and that r_0, j_0 and θ_0 are defined as in ((2.34)), ((2.48)) and ((2.47)), respectively. Then, for all $r \in (r_0, 1]$, we have*

$$\epsilon_{2,D}(n,r) < 0.237, \qquad \epsilon_{2,E}(n,r) < 0.266, \qquad \epsilon_{2,F}(n,r) < 0.266.$$

Proof: Making use of Lemmas 2.11.1 and 2.11.2 as well as of ((2.69)) and ((2.70)), and also noticing that $\phi^*(n,r,\rho)$ is increasing with respect to n, we infer

$$\begin{aligned}
\epsilon_{2,P}(n,r) &= \sqrt{\frac{g_P(n,r)}{2\pi}}\left(\sum_{j=0}^{j_0}\frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)}\right)\left(\int_{\theta_0}^{2\pi-\theta_0}\sup_{0\leqslant j\leqslant j_0}\left|\frac{P_{n,j}(re^{i\theta})}{\tilde{P}_{n,j}(r)}\right| d\theta\right)\\
&< \sqrt{\frac{24}{5\pi}}\left(\frac{1-r^n}{1-r}\right)^{3/2}\left(\sum_{j=0}^{j_0}\frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)}\right)\\
&\qquad\times\left(\frac{1-r}{1-r^n}\int_{1/3}^{3/2}\exp\left(-\phi^*(n,r,\rho)\right)d\rho+\pi\exp\left(-\phi^*(n,r,3/2)\right)\right)\\
&< \sqrt{\frac{24}{5\pi}}\left(\sum_{j=0}^{j_0}\frac{\tilde{P}_{n,j}(r)}{\tilde{P}_{n,0}(r)}\right)\\
&\qquad\times\left(\left(\frac{1}{1-r_0}\right)^{1/2}\int_{1/3}^{3/2}\exp\left(-\phi^*(n_0,r_0,\rho)\right)d\rho+\pi\left(\frac{1}{1-r_0}\right)^{3/2}\exp\left(-\phi^*(n_0,r_0,3/2)\right)\right).
\end{aligned}$$

Now we substitute $n_0 = 7000$ and[3] $r_0 = \exp(-\sqrt{\alpha/n_0}) \approx 0.987239$, and observe that $\frac{1}{1-r_0} \approx 78.3612$ and $\phi^*(n_0,r_0,3/2) \approx 14.5302$. Moreover, we use numerical integration to calculate

$$\int_{1/3}^{3/2}\exp\left(-\phi^*(n_0,r_0,\rho)\right)d\rho \approx 0.0177756 < \frac{4}{225}.$$

Therefore, we infer that

$$\begin{aligned}
\sqrt{\frac{24}{5\pi}}\left(\frac{1}{1-r_0}\right)^{1/2}&\int_{1/3}^{3/2}\exp\left(-\phi^*(n,r_0,\rho)\right)d\rho+\pi\left(\frac{1}{1-r_0}\right)^{3/2}\exp\left(-\phi^*(n,r_0,3/2)\right)\\
&< \sqrt{\frac{24}{5\pi}}\left(78.3612^{1/2}\times\frac{4}{225}+78.3612^{3/2}\pi\times e^{-14.5302}\right)\\
&\approx 0.195842 < \frac{1}{5}.
\end{aligned}$$

If this inequality is combined with ((2.65)) and ((2.66)), the proof is complete. □

[3] See again the remark after Lemma 2.9.2 for the meaning of the symbol $\approx$.

2.12 Concluding the Proof

Having finally obtained upper bounds for all the error terms, we combine them to derive the main result of this paper.

Theorem 2.12.1 *The Borwein Conjecture is true for all* $n > n_0 = 7000$.

Proof: For all $P \in \{D, E, F\}$ and all $m \in [n, (\deg P_n)/2]$, we let r_s be the saddle point defined in Lemma 2.5.1. When $n > n_0$, we can see that

$$\lambda = \frac{r_s - r_s^{n+1}}{1 - r_s} > \frac{e^{\sqrt{\alpha/n_0}} - e^{(n_0+1)\sqrt{\alpha/n_0}}}{1 - e^{\sqrt{\alpha/n_0}}} > 77.$$

Thus, from Lemma 2.8.1 we infer

$$\epsilon_{0,P}(n, m, r_s) < \frac{7\sqrt{2}}{\sqrt{3\pi\lambda}} + \operatorname{erfc}\sqrt{\frac{\lambda}{84}} < \frac{7\sqrt{2}}{\sqrt{231\pi}} + \operatorname{erfc}\sqrt{\frac{77}{84}} \approx 0.54321 < 0.544.$$

Also, $\lambda > 77$ allows us to conclude that

$$\left(1 + \frac{\sqrt{5}}{3\sqrt{3\lambda}}\right) < 1.05,$$

which results in explicit bounds for $\epsilon_{1,P}(n, r_s)$ in Lemma 2.9.4,

$$\begin{aligned}
\epsilon_{1,D}(n, r_s) &< 0.187 \times 1.05 < 0.197,\\
\epsilon_{1,E}(n, r_s) &< 0.043 \times 1.05 < 0.046,\\
\epsilon_{1,F}(n, r_s) &< 0.043 \times 1.05 < 0.046.
\end{aligned}$$

Remembering the estimations in Lemmas 2.10.2 and 2.11.3, we make a table of the upper bounds we have obtained so far:

P	$\epsilon_{0,P} \leqslant$	$\epsilon_{1,P} \leqslant$	$\epsilon_{2,P} \leqslant$	$\epsilon_{3,P} \leqslant$	Sum
D	0.544	0.197	0.237	0.004	0.982
E	0.544	0.046	0.266	0.008	0.864
F	0.544	0.046	0.266	0.008	0.864

TABLE 2.1: List of upper bounds for the quantities $\epsilon_{i,P}(n, r_s)$.

From this table we can finally conclude that

$$\epsilon_{0,P}(n, m, r_s) + \epsilon_{1,P}(n, r_s) + \epsilon_{2,P}(n, r_s) + \epsilon_{3,P}(n, r_s) < 1$$

holds for all $P \in \{D, E, F\}$ and $n > n_0$, confirming the truth of the Borwein Conjecture in this range. □

2.13 Computer verification for $n \leqslant 7000$

We have explicitly verified $[q^m]P_n(q) > 0$ for all $P \in \{A, B, C\}$, and all n and m with $1 \leqslant n \leqslant 7000$ and $0 \leqslant m \leqslant n^2$ by using a computer. The program itself is written in C, and it consists of the calculation of the coefficients of $(q;q)_{3n}/(q^3;q^3)_n$ by iterative multiplication; in each step, we multiply the current polynomial by an additional factor of $(1-q^{3j-2})(1-q^{3j-1})$. Each polynomial multiplication is further optimized into a series of additions and subtractions owing to the fact that the additional factor only has coefficients of 1 and -1.

The GMP library [Gt02] was used for exact large-integer arithmetic. The computation was run at Johannes Kepler University in Linz, on a computer with 32 Intel Xeon processors at 2GHz (of which only 10 are used). The running time was 53 hours, and used up to 150 gigabytes of memory for storing all the coefficients.

2.14 Discussion

There are two more Borwein Conjectures mentioned in [And95]: a “Second Borwein Conjecture" that also relates to modulus 3, and a “Third Borwein Conjecture" that relates to modulus 5.

Conjecture 2.14.1 (P. BORWEIN) Let the polynomials $\alpha_n(q)$, $\beta_n(q)$ and $\gamma_n(q)$ be defined by the relationship

$$\frac{(q;q)_{3n}^2}{(q^3;q^3)_n^2} = \alpha_n(q^3) - q\beta_n(q^3) - q^2\gamma_n(q^3). \tag{2.75}$$

Then these polynomials have non-negative coefficients.

Conjecture 2.14.2 (P. BORWEIN) Let the polynomials $\nu_n(q)$, $\phi_n(q)$, $\chi_n(q)$, $\psi_n(q)$ and $\omega_n(q)$ be defined by the relationship

$$\frac{(q;q)_{5n}}{(q^5;q^5)_n} = \nu_n(q^5) - q\phi_n(q^5) - q^2\chi_n(q^5) - q^3\psi_n(q^5) - q^4\omega_n(q^5), \tag{2.76}$$

Then these polynomials have non-negative coefficients.

Both these conjectures are still wide open. In particular, no reasonable formulas for the polynomials have been found so far. We remark that the comparison of ((2.1)) and ((2.75)) yields the relationship $\alpha_n(q) = A_n^2(q) + 2qB_n(q)C_n(q)$, so non-negativity for the coefficients of $\alpha_n(q)$ follows trivially from this paper.

Recall that for our proof we used the formulas for $A_n(q)$, $B_n(q)$ and $C_n(q)$ given in Theorem 2.1.2. As we mentioned, these formulas had apparently not caught much attention so far. It is rather a different type of formula that was found to be much more inspiring, namely (see [And95, Theorem 3.1])

$$A_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j+1)/2} \begin{bmatrix} 2n \\ n+3j \end{bmatrix}_q, \tag{2.77}$$

$$B_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j-5)/2} \begin{bmatrix} 2n \\ n+3j-1 \end{bmatrix}_q, \tag{2.78}$$

$$C_n(q) = \sum_{j\in\mathbb{Z}} (-1)^j q^{j(9j+7)/2} \begin{bmatrix} 2n \\ n+3j+1 \end{bmatrix}_q, \tag{2.79}$$

where we used again the standard notation for q-binomial coefficients. These are so much more imaginative because of their resemblance with a family of formulas appearing as generating functions for partitions with restricted hook differences in [And+87]. Andrews et al. had shown that

$$\sum_{j\in\mathbb{Z}}(-1)^j q^{jK\frac{j(\alpha+\beta)+\alpha-\beta}{2}}\begin{bmatrix} m+n \\ n-Kj \end{bmatrix}_q \tag{2.80}$$

is the generating function for certain partitions with restricted hook differences, with α, β, K, m, n being non-negative integers satisfying $\alpha+\beta<2K$ and $\beta-K\leqslant n-m\leqslant K-\alpha$. Indeed, the generating function in ((2.77)) is the "special case" of ((2.80)) in which $m=n$, $\alpha=5/3$, $\beta=4/3$ and $K=3$. Similar observations hold for $B_n(q)$ and $C_n(q)$. In other words, the result of Andrews et al. seems to produce a proof of the Borwein Conjecture, except for the small flaw that the choices of α and β are not integral, and thus not legitimate.

Bressoud [Bre96] extended the mystery by making the following much more general conjecture.
Conjecture 2.14.3 (BRESSOUD [BRE96, CONJECTURE 6]) Suppose that $m, n\in\mathbb{Z}^+$, α and β are positive rational numbers, and K is a positive integer such that αK and βK are integers. If $1\leqslant\alpha+\beta\leqslant 2K+1$ (with strict inequalities if $K=2$) and $\beta-K\leqslant n-m\leqslant K-\alpha$, then the polynomial

$$\sum_{j\in\mathbb{Z}}(-1)^j q^{j(K(\alpha+\beta)j+K(\alpha-\beta))/2}\begin{bmatrix} m+n \\ m+Kj \end{bmatrix}$$

has non-negative coefficients.

To this day, Bressoud's conjecture has only been proved when $\alpha,\beta\in\mathbb{Z}$ (corresponding to the result of Andrews et al. [And+87] mentioned above), and several infinite families of fractional parameters (see [Ber20a; BW05; Bre81; IKS99; War01; War03]). The connection to partitions with hook difference conditions lets one hope that a similar combinatorial interpretation may exist for the polynomials in the Borwein Conjecture, but to this day no such connection has been found.

Our approach for proving Theorem 2.12.1 has been analytic. The formulas that we just discussed, in particular the formulas ((2.77))–((2.79)) for $A_n(q)$, $B_n(q)$ and $C_n(q)$, are unsuitable for asymptotic approximation. The reason is that each dominating term in the sums ((2.77))–((2.79)) has order $O(4^n/n)$, whereas the actual order of magnitude of $A_n(q)$, $B_n(q)$ and $C_n(q)$ is trivially bounded above by $O(3^n)$. In other words, in the sums ((2.77))–((2.79)), there is a huge amount of cancellations going on, which are seemingly impossible to control in order to find reasonable asymptotic estimates. In contrast, only the first term in the formulas in Theorem 2.1.2 contributes to the sum, as the other terms are asymptotically negligible, as we have shown.

We also mention the result of Li [Li20], which proves the positivity of the sum

$$\sum_{m\equiv k \pmod{n+1}}[q^m]A_n(q)$$

for all k with $0\leqslant k\leqslant n$, and furthermore establishes the asymptotics of this sum as $2\cdot 3^n n^{-1}(1+o(1))$. This result is in line with our estimation: the central coefficient of $P_n(q)$ can be approximated by

$$\frac{P_{n,0}(1)}{\sqrt{2\pi g_P(n,1)}}=C\,3^n n^{-3/2}(1+o(1)).$$

For further work on the estimation of sums of coefficients of "Borwein-type polynomials" along arithmetic progressions, we refer the reader to Li and Yu [LY20].

We are in fact very optimistic that our analytic approach will have further implications. It seems that it is possible to adapt our approach for a proof of Conjectures 2.14.1 and 2.14.2. It remains to see whether these ideas may also finally lead to a full proof of Bressoud's Conjecture. Furthermore, we believe that they may also provide a basis for establishing open unimodality and log-concavity questions concerning polynomials given by products/quotients of factors of the form $1 - q^k$, as found for example in [CWW08].

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2.A Appendix: Auxiliary inequalities

This appendix contains several auxiliary inequalities used in the course of the proof. As their proofs are tedious, we put them here so as not to disturb the flow of the argument in the main text.

2.A.1 Approximation error by a Gaußian

This part of the appendix is dedicated to bounding the error in the approximation of a function by a Gaußian function.

Lemma 2.A.1 *Suppose that $w \in \mathbb{R}^+$. Then we have*

$$\int_0^{\frac{3}{4}} we^{-wx^2}\left(e^{wx^3}-1\right)\,dx < 1.1. \tag{2.81}$$

Proof: Using a Taylor expansion of e^{wx^3}, we write the integral as a sum involving the lower incomplete gamma function $\gamma(s,a) = \int_0^a e^{-x}x^{s-1}dx$:

$$\begin{aligned}\int_0^{\frac{3}{4}} we^{-wx^2}\left(e^{wx^3}-1\right)\,dx &= \sum_{k=1}^{\infty}\int_0^{\frac{3}{4}} \frac{w^{k+1}}{k!}e^{-wx^2}x^{3k}\,dx \\ &= \sum_{k=1}^{\infty}\frac{1}{2k!\,w^{(k-1)/2}}\gamma\left(\frac{3k+1}{2},\frac{9}{16}w\right).\end{aligned}$$

We denote the summand by

$$u(k,w) := \frac{1}{2k!\,w^{(k-1)/2}}\gamma\left(\frac{3k+1}{2},\frac{9}{16}w\right),$$

and attempt to bound the summand from above.

- For $k = 1$, $u(k,w) = u(1,w)$ can be bounded above by $\frac{1}{2}\Gamma(2) = \frac{1}{2}$.

- For $k \geqslant 2$, we first note that $\lim_{w\to 0} u(k,w) = \lim_{w\to+\infty} u(k,w) = 0$. This implies that the maximum value of $u(k,w)$ on $w \in \mathbb{R}^+$ occurs at a point where $\frac{\partial u(k,w)}{\partial w} = 0$.

  By taking the derivative, we see that any such point w_0 satisfies

$$\gamma\left(\frac{3k+1}{2}, \frac{9}{16}w_0\right) = \frac{2e^{-9w_0/16}\left(\frac{3}{4}\sqrt{w}\right)^{3k+1}}{k-1}.$$

  By substituting this back into the expression for $u(k,w)$, we infer that

$$\begin{aligned}\sup_{w\geqslant 0} u(k,w) &\leqslant \sup_{w\geqslant 0} \frac{1}{2k!\, w^{(k-1)/2}} \frac{2e^{-9w/16}\left(\frac{3}{4}\sqrt{w}\right)^{3k+1}}{k-1} \\ &= \sup_{w\geqslant 0} \frac{e^{-9w/16} w^{k+1}\left(\frac{3}{4}\right)^{3k+1}}{k!\,(k-1)}.\end{aligned}$$

  Another derivative with respect to w shows that this supremum occurs when $w = \frac{16}{9}(k+1)$, giving our final bound for $u(w,k)$:

$$\begin{aligned}\sup_{w\geqslant 0} u(k,w) &\leqslant \frac{\left(\frac{3}{4}\right)^{k-1}(k+1)^{k+1}}{k!e^{k+1}(k-1)} \\ &< \frac{\left(\frac{3}{4}\right)^{k-1}\sqrt{k+1}}{(k-1)\sqrt{2\pi}},\end{aligned} \tag{2.82}$$

  where the last step used Stirling's approximation $n^n < \frac{n!e^n}{\sqrt{2\pi n}}$.

Directly using the upper bound ((2.82)), we get

$$\sum_{k=1}^{\infty} u(k,w) < \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \sum_{k=2}^{\infty} \frac{\left(\frac{3}{4}\right)^{k-1}\sqrt{k+1}}{(k-1)} \approx 1.60608,$$

which is worse than what we claimed. Instead, we use ((2.82)) for the terms with $k > 10$, and conclude that

$$\sum_{k=11}^{\infty} u(k,w) < \frac{1}{\sqrt{2\pi}} \sum_{k=11}^{\infty} \frac{\left(\frac{3}{4}\right)^{k-1}\sqrt{k+1}}{(k-1)} \approx 0.027469 < 0.03.$$

As for the leftover terms where $2 \leqslant k \leqslant 10$, we first give a crude bound for large w by noticing that

$$u(k,w) = \frac{1}{2k!\, w^{(k-1)/2}}\gamma\left(\frac{3k+1}{2}, \frac{9}{16}w\right) < \frac{1}{2k!\, w^{(k-1)/2}}\Gamma\left(\frac{3k+1}{2}\right).$$

This inequality implies that if $w \geqslant 25$, then we have

$$\sum_{k=2}^{10} u(k,w) < \sum_{k=2}^{10} \frac{1}{2k!\, 5^{k-1}}\Gamma\left(\frac{3k+1}{2}\right) \approx 0.4446.$$

The interval $[0, 25]$ is treated using the same method as in Lemma 2.A.9, and the resulting upper bound is approximately $0.5677 < 0.57$.

Combining all the above arguments, we obtain

$$\int_0^{\frac{3}{4}} we^{-wx^2}\left(e^{wx^3}-1\right)\,dx = \sum_{k=1}^{\infty} u(k,w) < \frac{1}{2} + 0.03 + 0.57 = 1.1.$$

□

Lemma 2.A.2 *Suppose that $x_0 > 0$ and $f \in C^3([-x_0, x_0]; \mathbb{C})$ satisfy $f(x) = -gx^2/2 + O(|x|^3)$ for some $g \in \mathbb{R}^+$. Let $h = \sup_{|x|\leqslant x_0} |f'''(x)|$. Suppose further that $x_0 < \frac{9g}{4h}$. Then we have*

$$\left|\sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{f(x)}\,dx - 1\right| \leqslant \operatorname{erfc}(x_0\sqrt{g/2}) + 1.1 \times \frac{2\sqrt{2}}{3\sqrt{\pi}}\frac{h}{g^{3/2}}.$$

Proof: Let $R_2(x) = f(x) + gx^2/2$. Taylor's theorem implies that

$$|R_2(x)| \leqslant \frac{h}{6}|x|^3.$$

We split the integral as follows:

$$\begin{aligned}\int_{-x_0}^{x_0} e^{f(x)}\,dx &= \int_{-x_0}^{x_0} e^{-gx^2/2}\,dx + \int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{R_2(x)}-1\right)\,dx \\ &= \frac{\sqrt{2\pi}}{\sqrt{g}}(1-\operatorname{erfc}(x_0\sqrt{g/2})) + \int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{R_2(x)}-1\right)\,dx.\end{aligned}$$

Therefore we have

$$\begin{aligned}\left|\sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{f(x)}\,dx - 1\right| &\leqslant \operatorname{erfc}(x_0\sqrt{g/2}) + \sqrt{\frac{g}{2\pi}}\left|\int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{R_2(x)}-1\right)\,dx\right| \\ &< \operatorname{erfc}(x_0\sqrt{g/2}) + \sqrt{\frac{2g}{\pi}}\int_0^{\frac{9g}{4h}} e^{-gx^2/2}\left(e^{hx^3/6}-1\right)\,dx.\end{aligned}$$

□

The last integral is then bounded using Lemma 2.A.1 by taking $w = 9g^3/(2h^2)$, and making the substitution $x \mapsto (hx)/(3g)$.

Lemma 2.A.3 *Suppose that $u, v \in \mathbb{R}^+$. Then we have*

$$\int_0^{\frac{3}{4\sqrt{2}}} we^{-wx^2}\left(e^{wx^4}-1\right)\,dx < \frac{1}{3\sqrt{3}}. \tag{2.83}$$

Proof: Using the Taylor expansion of e^{wx^4}, we write the integral as a sum involving the lower incomplete gamma function $\gamma(s,a) = \int_0^a e^{-x}x^{s-1}dx$,

$$\begin{aligned}\int_0^{\frac{3}{4\sqrt{2}}} we^{-wx^2}\left(e^{wx^4}-1\right)\,dx &= \sum_{k=1}^{\infty}\int_0^{\frac{3}{4\sqrt{2}}} \frac{w^{k+1}}{k!}e^{-wx^2}x^{4k}\,dx \\ &= \sum_{k=1}^{\infty}\frac{1}{2k!w^{(2k-1)/2}}\gamma\left(\frac{4k+1}{2}, \frac{9}{32}w\right).\end{aligned}$$

We denote the summand by

$$u(k,w) := \frac{1}{2k!w^{(2k-1)/2}}\gamma\left(\frac{4k+1}{2}, \frac{9}{32}w\right),$$

and attempt to bound the summand from above. We first note that

$$\lim_{w\to 0} u(k,w) = \lim_{w\to +\infty} u(k,w) = 0.$$

This means that the maximum value of $u(k,w)$ on $w \in \mathbb{R}^+$ occurs at a point where $\frac{\partial u(k,w)}{\partial w} = 0$. By taking a derivative, we can see any such point w_0 satisfies

$$\gamma\left(\frac{4k+1}{2}, \frac{9}{32}w_0\right) = \frac{2e^{-9w_0/32}\left(\frac{9}{32}w_0\right)^{(4k+1)/2}}{2k-1}.$$

substituting it back into the expression of $u(k,w)$, we are able to infer that

$$\begin{aligned}\sup_{w\geqslant 0} u(k,w) &\leqslant \sup_{w\geqslant 0} \frac{1}{2k!w^{(k-1)/2}} \frac{2e^{-9w/32}\left(\frac{9}{32}w\right)^{(4k+1)/2}}{2k-1} \\ &= \sup_{w\geqslant 0} \frac{e^{-9w/32}w^{k+1}\left(\frac{9}{32}\right)^{(4k+1)/2}}{k!(2k-1)}.\end{aligned}$$

Another derivative with respect to w shows that this supremum occurs when $w = \frac{32}{9}(k+1)$, giving our final bound for $u(w,k)$:

$$\begin{aligned}\sup_{w\geqslant 0} u(k,w) &\leqslant \frac{\left(\frac{9}{32}\right)^{k-1/2}(k+1)^{k+1}}{k!e^{k+1}(2k-1)} \\ &< \frac{\left(\frac{9}{32}\right)^{k-1/2}\sqrt{k+1}}{(2k-1)\sqrt{2\pi}},\end{aligned} \tag{2.84}$$

where the last step used Stirling's approximation $n^n < \frac{n!e^n}{\sqrt{2\pi n}}$.

Similar to the proof of Lemma 2.A.1, we use ((2.84)) on the terms with $k \geqslant 2$, and conclude that

$$\sum_{k=2}^{\infty} u(k,w) < \frac{1}{\sqrt{2\pi}} \sum_{k=2}^{\infty} \frac{\left(\frac{9}{32}\right)^{k-1/2}\sqrt{k+1}}{(2k-1)} \approx 0.04303 < 0.0431.$$

As for the term $u(1,w)$, we first note that

$$u(1,w) = \frac{\gamma(5/2, 9w/32)}{2\sqrt{w}} < \frac{\Gamma(5/2)}{2\sqrt{w}} = \frac{3\sqrt{\pi}}{8\sqrt{w}},$$

therefore $u(1,w) < \frac{1}{8}$ if $w \geqslant 9\pi$. The interval $[0, 9\pi]$ is treated using the same method as in Lemma 2.A.9, and the resulting upper bound is approximately $0.14875 < 0.1488$.

Combining all the above arguments, we conclude that

$$\int_0^{\frac{3}{4\sqrt{2}}} we^{-wx^2}\left(e^{wx^4}-1\right)\,dx = \sum_{k=1}^{\infty} u(k,w) < 0.1488 + 0.0431 = 0.1919 < \frac{1}{3\sqrt{3}}.$$

□

Lemma 2.A.4 *Suppose that $x_0 > 0$ and that $f \in C^4([-x_0, x_0])$ is an even function that satisfies $f(x) = -gx^2/2 + O(|x|^4)$ for some $g \in \mathbb{R}^+$. Let $h = \sup_{|x|\leqslant x_0} |f^{(4)}(x)|$. Suppose further that $x_0^2 < \frac{27g}{8h}$. Then we have*

$$\sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{f(x)}\,dx \leqslant 1 + \frac{\sqrt{2}}{9\sqrt{\pi}}\frac{h^{1/2}}{g}.$$

Proof: Let $R(x) = f(x) + gx^2/2$. Taylor's theorem implies that

$$|R(x)| \leqslant \frac{h}{24}|x|^4.$$

Similar to the proof of Lemma 2.A.2, we argue that

$$\begin{aligned}\sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{f(x)}\,dx &= 1 - \operatorname{erfc}(x_0\sqrt{g/2}) + \sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{R(x)}-1\right)\,dx \\ &\leqslant 1 + \sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{h|x|/24}-1\right)\,dx \\ &= 1 + \sqrt{\frac{2g}{\pi}}\int_0^{\sqrt{\frac{27g}{8h}}} e^{-gx^2/2}\left(e^{h|x|/24}-1\right)\,dx.\end{aligned}$$

□

The last integral is then bounded using Lemma 2.A.3 by taking $w = 6g^2/h$ and making the substitution $x \mapsto \sqrt{12g/h}\,x$.

2.A.2 Trigonometric sums and tail estimates

The second part of the appendix is dedicated to several inequalities that contribute to the proof of Lemma 2.11.1.

Lemma 2.A.5 *For all $r \in \mathbb{R}^+$ and $\theta \in \mathbb{R}$, we have*

$$\left|\frac{1 + re^{i\theta} + r^2e^{2i\theta}}{1 + r + r^2}\right| \leqslant \exp\left(-\frac{2r}{1+r^2}\sin^2(\theta/2)\right). \tag{2.85}$$

Proof: It is straightforward to calculate

$$\left|1 + re^{i\theta} + r^2e^{2i\theta}\right|^2 = 1 + (2-4s)r + (3 - 16s + 16s^2)r^2 + (2-4s)r^3 + r^4,$$

where $s = \frac{1}{2}(1-\cos\theta) = \sin(\theta/2)^2 \in [0,1]$.

We claim that

$$\left|\frac{1 + re^{i\theta} + r^2e^{2i\theta}}{1 + r + r^2}\right|^2 \leqslant \left(\frac{1 - rs + r^2}{1 + rs + r^2}\right)^2 \leqslant \exp\left(-\frac{4rs}{1+r^2}\right).$$

The first inequality is proved by the algebraic manipulation

$$(1+r+r^2)^2(1-rs+r^2)^2-(1+rs+r^2)^2\left(1+(2-4s)r+(3-16s+16s^2)r^2+(2-4s)r^3+r^4\right)$$
$$=4r^2s(1-s)\left((1+r^2)(2-r+r^2+7rs)+4r^2s^2\right)\geqslant 0,$$

while the second inequality can be obtained by taking $x=\frac{2rs}{1+r^2}$ in the inequality $\frac{1-x/2}{1+x/2}\leqslant e^{-x}$, which holds for all $x\in[0,1]$. □

Lemma 2.A.6 *Let $r\in\mathbb{R}^+$ and $b\geqslant 2$. Then we have*

$$\frac{(1-r^{b+1})(1-r^{b-1})}{r^{b-1}(b^2-1)(1-r)^2}\geqslant\frac{(1+r^{b/3})(1+r^b)}{2(r^{b/3}+r^b)}.$$

Proof: Let $z=\frac{b}{2}\log r$. The lemma is equivalent to

$$\frac{\sinh(z+z/b)\sinh(z-z/b)}{(b^2-1)\sinh^2(z/b)}\geqslant\frac{\cosh(z/3)\cosh z}{\cosh(2z/3)}. \tag{2.86}$$

When $b=2$, the difference between the two sides of ((2.86)) is

$$\frac{\sinh(3z/2)}{3\sinh(z/2)}-\frac{\cosh(z/3)\cosh z}{\cosh(2z/3)}$$
$$=\frac{(\cosh(z/3)-1)^2(2\cosh(z/3)+1)(8\cosh^2(z/3)+6\cosh(z/3)-1)}{3\cosh(2z/3)}\geqslant 0.$$

We now proceed to prove that the left-hand side of ((2.86)), viewed as a function with respect to b and fixed z, is increasing. To this end, we compute its derivative as

$$2\frac{(b^2-1)z\cosh(z/b)\sinh^2 z-b^3\sinh(z/b)\sinh(z-z/b)\sinh(z+z/b)}{b^2(b^2-1)^2\sinh^3(z/b)},$$

so it suffices to prove that

$$(b^2-1)z\cosh(z/b)\sinh^2 z\cosh(z/b)\sinh^2(z)\geqslant b^3\sinh(z/b)\sinh(z-z/b)\sinh(z+z/b),$$

or equivalently,

$$\frac{\sinh(2z/b)\sinh^2(z)}{(2z/b)z^2}\geqslant\frac{\sinh(z/b)^2\sinh(z-z/b)\sinh(z+z/b)}{(z/b)^2(z-z/b)(z+z/b)}.$$

Taking the logarithm on both sides, and defining $f(x):=\log\frac{\sinh x}{x}$ and $f(0):=0$, we arrive at another equivalent form,

$$f(z+z/b)+f(z-z/b)-2f(z)+2f(z/b)-f(2z/b)-f(0)\leqslant 0.$$

The left-hand side can be written as a triple integral,

$$f(z+z/b)+f(z-z/b)-2f(z)+2f(z/b)-f(2z/b)-f(0)=\iiint\limits_{[0,z/b]^2\times[z/b,z]}f'''(\gamma+\alpha-\beta)d\alpha\,d\beta\,d\gamma,$$

and we conclude the proof by noting that

$$f'''(x) = 2(\cosh x(\sinh x)^{-3} - x^{-3}) \leqslant 0. \qquad \square$$

The following inequality gives a simple rational lower bound for the Chebyshev polynomials of the first kind $T_n(x)$, defined by $T_n(\cos\theta) = \cos n\theta$.

Lemma 2.A.7 *For all $x \in [-1, 1]$ and all $n \in \mathbb{Z}^+$, we have*

$$T_n(x) \geqslant \frac{-n^2(1-x)(2x+3) + 3(1+x)}{n^2(1-x) + 3(1+x)}.$$

Proof: If $n = 1$, then both sides are equal to x. From now on we assume $n \geqslant 2$.

If $-1 \leqslant x \leqslant 1 - \frac{3}{n^2}$, then we have

$$\frac{-n^2(1-x)(2x+3) + 3(1+x)}{n^2(1-x) + 3(1+x)} \leqslant -1 \leqslant T_n(x).$$

If $1 - \frac{3}{n^2} \leqslant x \leqslant 1$, then we write $\theta = \frac{n}{2}\arccos x$, so that

$$0 \leqslant \theta \leqslant n \arcsin\sqrt{\frac{3}{2n^2}}.$$

The two sides of the inequalities can be rewritten as

$$T_n(x) = \cos 2\theta = 1 - 2\sin^2\theta$$

and

$$\begin{aligned}\frac{-n^2(1-x)(2x+3) + 3(1+x)}{n^2(1-x) + 3(1+x)} &= 1 - \frac{n^2(2x+4)}{n^2 + 3\frac{1+x}{1-x}} \\ &= 1 - \frac{2\cos(2\theta/n) + 4}{1 + 3n^{-2}\cot^2(\theta/n)} \\ &= 1 - \frac{6 - 4\sin^2(\theta/n)}{1 + 3n^{-2}\cot^2(\theta/n)}.\end{aligned}$$

Thus it suffices to prove that

$$\sin^2\theta(1 + 3n^{-2}\cot^2(\theta/n)) \leqslant 3 - 2\sin^2(\theta/n)$$

for all $n \geqslant 2$ and $\theta \in [0, n\arcsin\sqrt{\frac{3}{2n^2}}]$.

For the last inequality, we make use of the inequalities, valid at least for $x \in (0, \pi/2)$ (The first one is a consequence of the elementary inequality $\cos x \geqslant 1 - x^2/2 + x^4/4! - x^6/6!$, the second one is a consequence of the fact that the Taylor expansion of $\cot x - \frac{1}{x}$ only has negative terms).

$$\sin^2 x \leqslant x^2 - \frac{x^4}{3} + \frac{2x^6}{45},$$

$$\cot x \leqslant \frac{1}{x} - \frac{x}{3} - \frac{x^3}{45},$$

to conclude that

$$\begin{aligned}
&3 - 2\sin^2(\theta/n) - \sin^2\theta(1 + 3n^{-2}\cot^2(\theta/n)) \\
&\qquad \geqslant 3 - 2\left(\frac{\theta^2}{n^2} - \frac{\theta^4}{3n^4} + \frac{2\theta^6}{45n^6}\right) - \left(\theta^2 - \frac{\theta^4}{3} + \frac{2\theta^6}{45}\right)\left(1 + \frac{3}{n^2}\left(\frac{n}{\theta} - \frac{\theta}{3n} - \frac{\theta^3}{45n^2}\right)^2\right) \\
&\qquad = \theta^4\left(\frac{(n^2-1)(7n^2-3)}{15n^4} - \frac{(n^2-2)(2n^4-3)}{45n^6}\theta^2 - \frac{6n^4-10n^2+1}{675n^8}\theta^4\right. \\
&\qquad\qquad \left. - \frac{4n^2-1}{2025n^8}\theta^6 - \frac{2}{30375n^8}\theta^8\right).
\end{aligned}$$

The last factor is clearly decreasing with respect to θ when $n \geqslant 2$, so we proceed to find an upper bound for θ. We note that

$$\frac{d}{dn} n \arcsin\sqrt{\frac{3}{2n^2}} = \arcsin\sqrt{\frac{3}{2n^2}} - \frac{1}{\sqrt{\frac{2n^2}{3} - 1}},$$

and after substituting $\phi = \arcsin\sqrt{\frac{3}{2n^2}}$ we see that the derivative is equal to $\phi - \tan\phi < 0$. So $n \arcsin\sqrt{\frac{3}{2n^2}}$ is decreasing with respect to n. This implies that we always have

$$0 \leqslant \theta \leqslant n \arcsin\sqrt{\frac{3}{2n^2}} \leqslant 2\arcsin\sqrt{\frac{3}{8}} < \sqrt{\frac{15}{8}}.$$

Using this bound, we conclude that

$$\begin{aligned}
&3 - 2\sin^2(\theta/n) - \sin^2\theta(1 + 3n^{-2}\cot^2(\theta/n)) \\
&\qquad \geqslant \theta^4\left(\frac{(n^2-1)(7n^2-3)}{15n^4} - \frac{(n^2-2)(2n^4-3)}{45n^6}\theta^2 - \frac{6n^4-10n^2+1}{675n^8}\theta^4\right. \\
&\qquad\qquad \left. - \frac{4n^2-1}{2025n^8}\theta^6 - \frac{2}{30375n^8}\theta^8\right) \\
&\qquad \geqslant \theta^4\left(\frac{(n^2-1)(7n^2-3)}{15n^4} - \frac{(n^2-2)(2n^4-3)}{45n^6}\frac{15}{8} - \frac{6n^4-10n^2+1}{675n^8}\left(\frac{15}{8}\right)^2\right. \\
&\qquad\qquad \left. - \frac{4n^2-1}{2025n^8}\left(\frac{15}{8}\right)^3 - \frac{2}{30375n^8}\left(\frac{15}{8}\right)^4\right) \\
&\qquad = \frac{15\theta^4}{2^{17}n^8}\left(512n^4(n^2-4)(7n^2-2) + 6480(n^2-1)(2n^2+1) + 160n^4 + 6395\right) \\
&\qquad \geqslant 0. \qquad \square
\end{aligned}$$

Lemma 2.A.8 *Let $a, b \in \mathbb{Z}^+$ such that $b \geqslant 2$, and $r \in [0,1]$. Then we have*

$$\sum_{m=a}^{a+b-1} r^{m-a} \sin^2(m\theta/2) \geqslant \frac{1}{2}\frac{1-r^b}{1-r}\left(1-\sqrt{\frac{1+\kappa\frac{(1+r^b)^2}{(1-r^b)^2}\tan^2(\theta/2)}{1+\kappa\frac{(1+r)^2}{(1-r)^2}\tan^2(\theta/2)}}\right),$$

where

$$\kappa = \frac{(1-r^b)(1-r^{b/3})}{(1+r^b)(1+r^{b/3})}.$$

Proof: This sum has a closed form,

$$\begin{aligned}\sum_{m=a}^{a+b-1} & r^{m-a}\sin(m\theta/2)^2 \\ &= \frac{1}{2}\left(\frac{1-r^b}{1-r} - \frac{(\cos a\theta - r\cos((a-1)\theta)) - r^b(\cos(a+b)\theta - r\cos((a+b-1)\theta))}{1-2r\cos\theta+r^2}\right) \\ &= \frac{1}{2}\left(\frac{1-r^b}{1-r} - \frac{(\cos a\theta - r^b\cos(a+b)\theta)(1-r\cos\theta) - (\sin a\theta - r^b\sin(a+b)\theta)\sin\theta}{1-2r\cos\theta+r^2}\right).\end{aligned}$$

We use the Cauchy–Schwarz inequality, observe that

$$(1-r\cos\theta)^2 + (r\sin\theta)^2 = 1-2r\cos\theta+r^2$$

and

$$(\cos a\theta - r^b\cos(a+b)\theta)^2 + (\sin a\theta - r^b\sin(a+b)\theta)^2 = 1-2r^b\cos b\theta + r^{2b},$$

to arrive at

$$\sum_{m=a}^{b-1} r^{m-a}\sin(m\theta/2)^2 \geqslant \frac{1}{2}\left(\frac{1-r^b}{1-r} - \sqrt{\frac{1-2r^b\cos b\theta + r^{2b}}{1-2r\cos\theta+r^2}}\right). \tag{2.87}$$

Comparing ((2.87)) with the claims of this lemma, we see that it suffices to prove that

$$\frac{1-2r^b\cos b\theta + r^{2b}}{1-2r\cos\theta+r^2} \leqslant \frac{(1-r^b)^2+\kappa(1+r^b)^2\tan^2(\theta/2)}{(1-r)^2+\kappa(1+r)^2\tan^2(\theta/2)}.$$

By routine manipulation, the above inequality is equivalent to

$$\cos\theta - \cos b\theta \leqslant \frac{(1-\kappa)(1-r^{b-1})(1-r^{b+1})\sin^2\theta}{r^{b-1}\left((1-r)^2(1+\cos\theta)+\kappa(1+r)^2(1-\cos\theta)\right)}. \tag{2.88}$$

Here, Lemma 2.A.7 implies the inequality

$$\cos\theta - \cos b\theta \leqslant \frac{(b^2-1)\sin^2\theta}{(1+\cos\theta)+b^2(1-\cos\theta)/3}. \tag{2.89}$$

Comparing ((2.88)) and ((2.89)), we see that it remains to show that

$$\frac{r^{b-1}\left((1-r)^2(1+\cos\theta)+\kappa(1+r)^2(1-\cos\theta)\right)}{(1-\kappa)(1-r^{b-1})(1-r^{b+1})} \leqslant \frac{(1+\cos\theta)+b^2(1-\cos\theta)/3}{b^2-1}. \tag{2.90}$$

This is an immediate consequence of Lemma 2.A.6 and the inequality

$$\kappa \leqslant \frac{b^2}{3}\frac{(1-r)^2}{(1+r)^2}. \tag{2.91}$$

Equation ((2.91)) can be directly verified for $b = 2$. If $b \geqslant 3$, we write $r = e^{-x/2}$, so that the inequality is equivalent to

$$\frac{\tanh(bx)\tanh(bx/3)}{(\tanh x)^2} \leqslant \frac{b^2}{3}.$$

This follows finally from the fact that $\tanh x/x$ is decreasing on $\mathbb{R}^+$. □

2.A.3 Miscellaneous Inequalities

Lemma 2.A.9 *For all $z = re^{i\theta} \in \mathbb{C}$ such that $0 \leqslant r \leqslant 1$ and $|\theta| \leqslant \frac{1}{3}\frac{(-\log r)}{(1-r)}$, we have*

$$\left|\frac{1}{1+z+z^2}\right| < 1.002, \tag{2.92}$$

$$\left|\frac{(1-z)^2}{1+z+z^2}\right| < 1.005, \tag{2.93}$$

$$\left|\frac{(1-z^2)(1+7z+z^2)}{(1+z+z^2)^3}\right| < \frac{7}{5}, \tag{2.94}$$

$$\left|\frac{1+12z-12z^2-56z^3-12z^4+12z^5+z^6}{(1+z+z^2)^4}\right| < \frac{5}{3}. \tag{2.95}$$

Proof: Let S be the region

$$\{z = re^{i\theta} \in \mathbb{C} \mid 0 \leqslant r \leqslant 1,\ |\theta| \leqslant \frac{1}{3}\frac{(-\log r)}{(1-r)}\}.$$

All the rational functions on the left-hand sides of the inequalities are holomorphic on S, so the maximum modulus principle means it suffices to prove the inequalities on the boundary

$$\partial S = \left\{z = re^{i\theta} \in \mathbb{C} \,\middle|\, 0 < r < 1,\ -\pi \leqslant \theta \leqslant \pi,\ |\theta| = \frac{1}{3}\frac{(-\log r)}{(1-r)}\right\} \cup \left\{e^{i\theta} \,\middle|\, |\theta| \leqslant \frac{1}{3}\right\}.$$

The proof is done in a uniform way for all four rational functions (denoted by f in the subsequent arguments): let $g_1, g_2, g_3 : [0,1] \to \mathbb{C}$ be a three-part parametrization of ∂S given by

$$g_1(x) = \exp\left(-3\pi x + \frac{-\pi x}{(1-e^{3\pi x})}i\right)$$

$$g_2(x) = \exp\left(-3\pi x - \frac{-\pi x}{(1-e^{3\pi x})}i\right)$$

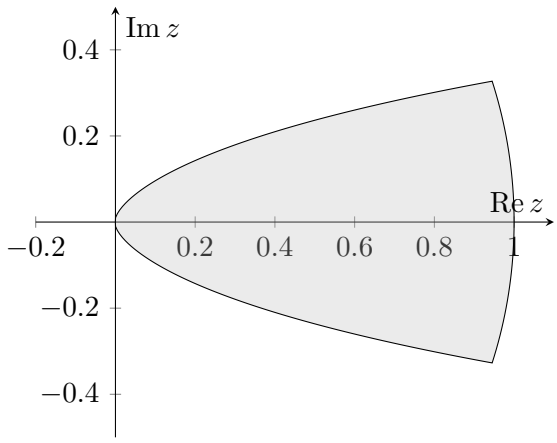

FIGURE 2.2: Illustration of the region S (shaded).

$$g_3(x) = \exp\left(\frac{2x-1}{3}i\right).$$

We choose $N = 10^6$ points in $[0,1]$, namely $0, 1/N, \ldots, (N-1)/N$, and argue that

$$|f(z)| \leqslant \max_{k=1}^{3}\left(\max_{j=0}^{N-1}|f(g_k(j/N))| + \frac{1}{N}\sup_{x\in[0,1]}|f'(g_k(x))|\,|g_k'(x)|\right)$$

holds for all $z \in \partial S$. Then we evaluate $\max_j |f(g_k(j/N))|$ using a computer, and prove trivial upper bounds for f', and $g_k'(k = 1, 2, 3)$:

- The derivative $f'(z)$ is a rational function with denominator equal to a power of $1 + z + z^2$. We note that $S \subset (-1/3, 1] + (-1/3, 1/3)i$ implies that $|1 + z + z^2| \geqslant \sqrt{37}/9 > 2/3$ for all $z \in S$, and use this to bound the denominators; on the other hand we use trivial triangle inequalities to control the numerators, and combine them to obtain upper bounds for f'.
- The derivatives of $g_1(x)$ and $g_2(x)$ can be bounded by $e^{-3\pi x}|3\pi + \pi i| = \pi\sqrt{10}e^{-3\pi x} \leqslant 10$.
- We obviously have $|g_3'(x)| = \frac{2}{3}$ for all x. □

By combining these bounds we conclude the proof.

The next lemma deals with inequalities between sums of the form $\sum_{k=1}^{n} k^a r^k$.

Lemma 2.A.10 *For all $n \in \mathbb{Z}^+$ and all $r \in (0, 1]$, we have*

$$3r^2\left(\sum_{k=1}^{n} k^2 r^k\right) \geqslant \left(\sum_{k=1}^{n} r^k\right)^3, \tag{2.96}$$

$$(r+1)\left(\sum_{k=1}^{n} r^k\right)^3 \geqslant r^2\left(\sum_{k=1}^{n} k^2 r^k\right), \tag{2.97}$$

$$(r^2+4r+1)\left(\sum_{k=1}^{n} r^k\right)\left(\sum_{k=1}^{n} k^2 r^k\right) \geqslant r(r+1)\left(\sum_{k=1}^{n} k^3 r^k\right), \tag{2.98}$$

$$(r^2+4r+1)^2\left(\sum_{k=1}^{n}k^2r^k\right)^3 \geqslant (r+1)^3\left(\sum_{k=1}^{n}k^3r^k\right)^2\left(\sum_{k=1}^{n}r^k\right), \tag{2.99}$$

$$(r^2+10r+1)\left(\sum_{k=1}^{n}r^k\right)^2\left(\sum_{k=1}^{n}k^2r^k\right) \geqslant r^2\left(\sum_{k=1}^{n}k^4r^k\right), \tag{2.100}$$

$$(r^2+10r+1)\left(\sum_{k=1}^{n}k^2r^k\right)^2 \geqslant (r+1)\left(\sum_{k=1}^{n}k^4r^k\right)\left(\sum_{k=1}^{n}r^k\right). \tag{2.101}$$

Proof: For simplicity of notation, we use X_m to denote the sum $\sum_{k=1}^{n}k^mr^k$. The reader should observe that, for fixed m, the sum X_m can be evaluated into a rational function in r and r^n by applying the binomial theorem.

The first inequality is proved by noticing that the coefficient $[r^k](3r^2X_2-X_0^3)$ is equal to $3(k-2)^2-\binom{k-1}{2}>0$ for $3\leqslant k\leqslant n+2$, and is negative for $n+3\leqslant k\leqslant 3n$. Moreover, the sum of the coefficients is equal to

$$3\sum_{k=1}^{n}k^2-n^3=\frac{n(3n+1)}{2}>0.$$

So we have

$$3r^2\left(\sum_{k=1}^{n}k^2r^k\right)-\left(\sum_{k=1}^{n}r^k\right)^3 \geqslant lr^{n+2}-lr^{n+3}+\frac{n(3n+1)}{2}r^{n+3}>0,$$

where l is the sum of all positive coefficients in $3r^2X_2-X_0^3$.

In order to prove the other inequalities, we give explicit formulas for the coefficients of the differences between both sides in those inequalities. More explicitly, after some tedious but routine calculations, we arrive at the following results:

- For ((2.97)), we have

$$(r+1)X_0^3-r^2X_2=r^{n+3}\sum_{k=0}^{2n-1}a_kr^k,$$

  where $a_k=(n+k+1)^2-3(k+1)^2$ for $0\leqslant k<n$, and $a_k=(2n-k-1)^2$ for $n\leqslant k<2n$.

- For ((2.98)), we have

$$(r^2+4r+1)X_0X_2-r(r+1)X_3=r^{n+2}\sum_{k=0}^{n}b_kr^k,$$

  where $b_0=n(n+1)^2-1$, $b_n=n^2$, $b_k=n(n+1)(2n+1)-(2k+1)(k^2+k+1)$ for $0<k<n$.

- For ((2.99)), we have

$$(r^2+4r+1)^2X_2^3-(r+1)^3X_0X_3^2=\frac{nr^{n+3}}{210}\sum_{k=0}^{2n+1}c_kr^k,$$

where

$$c_k=\begin{cases}-12k^7-42k^6n-84k^6+168k^5n^2+126k^5n-294k^5+420k^4n^2+315k^4n-630k^4 \\ \quad +1400k^3n^2+1680k^3n-798k^3+1680k^2n^2+2247k^2n-546k^2+1372kn^2+1974kn \\ \quad -156k+420n^2+630n, & 0\leqslant k< \\ 114n^7+462n^6+1211n^5+1470n^4+301n^3-252n^2-156n, & k=n, \\ 12k^7+42k^6n+84k^6-168k^5n^2-126k^5n+294k^5-420k^4n^2-315k^4n+630k^4 \\ \quad -840k^3n^4-1680k^3n^3-2240k^3n^2-1680k^3n+798k^3+3276k^2n^5+7560k^2n^4 \\ \quad +5250k^2n^3-420k^2n^2-1953k^2n+546k^2-3024kn^6-6468kn^5-3360kn^4+840kn^3 \\ \quad -28kn^2-1386kn+156k+816n^7+1512n^6+1372n^5+2100n^4+2114n^3 \\ \quad +588n^2-312n, & n<k\leqslant \\ 210n^5, & k=2n+\end{cases}$$

- For ((2.100)), we have

$$(r^2+10r+1)X_0^2X_2-r^2X_4=r^{n+3}\sum_{k=0}^{2n-1}d_kr^k,$$

where $d_k=n^4+4(k+1)n^3-2(k+1)^4+(6k+5)n^2+2(k+1)n$ for $0\leqslant k<n$, and $d_k=(2n-1-k)^2(2n^2+(k+1)^2)+2n(3n+1)(2n-1-k)+n^2$ for $n\leqslant k<2n$.

- For ((2.101)), we have

$$(r^2+10r+1)X_2^2-(r+1)X_0X_4=nr^{n+2}\sum_{k=0}^{n}e_kr^k,$$

where $e_k=n^3+2(n-k)(kn^2+(3k^2+4k+2)n+(k+1)^2(k+2))$.

It is easy to see that a_k, b_k, c_n, c_{2n+1}, d_k and e_k are non-negative. For the remaining c_k's, we distinguish two cases:

- $0\leqslant k<n$. Here we substitute $k=\lambda n$ with $0\leqslant\lambda<1$ to see that

$$\begin{aligned}c_k=&\left(-12\lambda^7-42\lambda^6+168\lambda^5\right)n^7+\left(-84\lambda^6+126\lambda^5+420\lambda^4\right)n^6+\left(-294\lambda^5+315\lambda^4+1400\lambda^3\right)n^5\\&+\left(-630\lambda^4+1680\lambda^3+1680\lambda^2\right)n^4+\left(-798\lambda^3+2247\lambda^2+1372\lambda\right)n^3+\left(-546\lambda^2+1974\lambda+420\right)n^2\\&+(630-156\lambda)n,\end{aligned}$$

and note that $0\leqslant\lambda<1$ implies that every coefficient above is non-negative.

- $n\leqslant k\leqslant 2n$. Similarly, we substitute $k=(2-\lambda)n$ to write

$$\begin{aligned} c_k = &\left(-12\lambda^7 + 210\lambda^6 - 1344\lambda^5 + 4200\lambda^4 - 5880\lambda^3 + 2940\lambda^2\right) n^7 \\ &+ \left(84\lambda^6 - 882\lambda^5 + 3360\lambda^4 - 3360\lambda^3 - 2520\lambda^2 + 3780\lambda\right) n^6 \\ &+ \left(-294\lambda^5 + 2625\lambda^4 - 7000\lambda^3 + 7770\lambda^2 - 4200\lambda + 2100\right) n^5 \\ &+ \left(630\lambda^4 - 3360\lambda^3 + 4620\lambda^2 + 840\lambda - 1260\right) n^4 + \left(-798\lambda^3 + 2835\lambda^2 - 1736\lambda + 630\right) n^3 \\ &+ \left(546\lambda^2 - 798\lambda\right) n^2 - 156\lambda n. \end{aligned}$$

In this case some of the coefficients (namely, the coefficients of n, n^2 and of n^4) are negative. However, by exploiting the fact that $n \geqslant 1$ and that

$$\begin{aligned} [n^5]c_k + [n^4]c_k &= -294\lambda^5 + 3255\lambda^4 - 10360\lambda^3 + 12390\lambda^2 - 3360\lambda + 840 \\ &= 840(1 - 2\lambda + 2\lambda^2)^2 + 7\lambda^2(810 - 520\lambda - 15\lambda^2 - 42\lambda^3) > 0, \\ [n^3]c_k + [n^2]c_k + [n^1]c_k &= -798\lambda^3 + 3381\lambda^2 - 2690\lambda + 630 \\ &= 523(1 - 2\lambda)^2 + (1 - \lambda)(798\lambda^2 - 491\lambda + 107) > 0, \end{aligned}$$ □

we can still directly conclude that $c_k \geqslant 0$. □

The following two inequalities are used in the proof of Lemma 2.11.2.

Lemma 2.A.11 *Suppose that* $0 < r \leqslant 1$, *and* $n \geqslant 1$. *Then we have*

$$\frac{(1-r^n)^2}{(1-r)^2} \geqslant \frac{\partial}{\partial r}\frac{1-r^n}{1-r} \geqslant \frac{(1-r^n)(1-r^{(n-1)/2})}{(1-r)^2}.$$

Proof: Direct calculation reveals that

$$\begin{aligned} \frac{\partial}{\partial r}\frac{1-r^n}{1-r} - \frac{(1-r^n)(1-r^{(n-1)/2})}{(1-r)^2} &= \frac{r^{n-1/2}}{(1-r)^2}\left(r^{-n/2} - r^{n/2} - n(r^{-1/2} - r^{1/2})\right), \\ \frac{(1-r^n)^2}{(1-r)^2} - \frac{\partial}{\partial r}\frac{1-r^n}{1-r} &= \frac{r^{n-1}}{(1-r)^2}\left(n(1-r) - r(1-r^n)\right). \end{aligned}$$

Therefore, the lemma follows from the elementary inequality

$$\frac{r(1-r^n)}{1-r} \leqslant n \leqslant \frac{r^{-n/2} - r^{n/2}}{r^{-1/2} - r^{1/2}}.$$ □

Lemma 2.A.12 *Suppose that* $n \geqslant 6924$, *and* $r \in (\exp(-\sqrt{\alpha/n}), 1]$ *with* $\alpha = 2/\sqrt{3}$. *Then we have*

$$\frac{(1-r^{n/12})(1-r^{(n-12)/24})}{(1-r)(1-r^n)} \geqslant 24.$$

Proof: First of all, the condition $n \geqslant 6924$ implies that $1 - r^{(n-12)/24} \geqslant 1 - r^{288}$, as well as $r > \exp(-\sqrt{\alpha/6924}) > e^{-1/72}$.

Noting that the function $\frac{1-r^{n/12}}{1-r^n}$ is increasing with respect to n, we conclude that

$$\frac{(1-r^{n/12})(1-r^{(n-12)/24})}{1-r^n} \geqslant \frac{(1-r^{n/12})(1-r^{288})}{1-r^n} \geqslant \frac{(1-r^{48})(1-r^{288})}{1-r^{576}} = \frac{1-r^{48}}{1+r^{288}}.$$

Thus it suffices to prove that $1 - r^{48} \geqslant 24(1-r)(1+r^{288})$ for $r \in (e^{-1/72}, 1]$. To this end, we

prove that $1-r^{48}-24(1-r)(1+r^{288})$ is decreasing on $(e^{-1/72},1]$ by calculating the derivative. We have

$$\begin{aligned}\frac{d}{dr}\left((1-r^{48})-24(1-r)(1+r^{288})\right) &= 24(1-2r^{48}+r^{288})-48(1-r)(r^{47}+144r^{287})\\ &\leqslant 24r^{48}(r^{-48}+r^{240}-2)\leqslant 24r^{48}\max\left(e^{2/3}+e^{-10/3}-2,1+1-2\right)=0,\end{aligned}$$

where we exploit the convexity of the function $r\mapsto r^{-48}+r^{240}-2$. □

The following inequality is used in the proof of Lemma 2.9.1.

Lemma 2.A.13 *Suppose* $0<a\leqslant b$, *and* $0<c\leqslant \pi/b$. *Then for all* $z\in\mathbb{C}$ *such that* $(\operatorname{Im} z)^2\leqslant(\operatorname{Re} z)^2+c^2$, *we have*

$$\left|\frac{\sinh(az)}{\sinh(bz)}\right|\leqslant\frac{\sin(ac)}{\sin(bc)}.$$

Proof: We make use of the infinite products

$$\sinh z = z\prod_{k=1}^{\infty}\left(1+\frac{z^2}{k^2\pi^2}\right)$$

and

$$\sin z = z\prod_{k=1}^{\infty}\left(1-\frac{z^2}{k^2\pi^2}\right).$$

We claim that under the assumptions of this lemma, we have

$$\left|\frac{k^2\pi^2+a^2z^2}{k^2\pi^2+b^2z^2}\right|\leqslant\frac{k^2\pi^2-a^2c^2}{k^2\pi^2-b^2c^2},$$

from which the lemma follows after taking the product over all $k\geqslant 1$.

In order to prove this inequality, we write $z^2=x+iy$ and $u=k\pi$, so that $x\geqslant -c^2$ and $ac\leqslant bc\leqslant u$. Now the absolute value can be written as

$$\left|\frac{u^2+a^2z^2}{u^2+b^2z^2}\right|=\sqrt{\frac{(u^2+a^2x)^2+a^4y^2}{(u^2+b^2x)^2+b^4y^2}},$$

and the inequality can be proved by the manipulation

$$\begin{aligned}\left((u^2+b^2x)^2+b^4y^2\right)(u^2-a^2c^2)^2-&\left((u^2+a^2x)^2+a^4y^2\right)(u^2-b^2c^2)^2\\ &=u^2(b^2-a^2)\left[(u^2-a^2c^2)((x+c^2)(u^2+b^2x)+b^2y^2)\right.\\ &\qquad\left.+(u^2-b^2c^2)((x+c^2)(u^2+a^2x)+a^2y^2)\right]\\ &\geqslant 0.\end{aligned}$$

□

3

An asymptotic approach to Borwein-type sign pattern theorems

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Abstract

The celebrated (First) Borwein Conjecture predicts that for all positive integers n the sign pattern of the coefficients of the "Borwein polynomial"

$$(1-q)(1-q^2)(1-q^4)(1-q^5)\cdots(1-q^{3n-2})(1-q^{3n-1})$$

is $+--+--\cdots$. It was proved by the first author in [*Adv. Math.* **394** (2022), Paper No. 108028]. In the present paper, we extract the essentials from the former paper and enhance them to a conceptual approach for the proof of "Borwein-like" sign pattern statements. In particular, we provide a new proof of the original (First) Borwein Conjecture, a proof of the Second Borwein Conjecture (predicting that the sign pattern of the square of the "Borwein polynomial" is also $+--+--\cdots$), and a partial proof of a "cubic" Borwein Conjecture due to the first author (predicting the same sign pattern for the cube of the "Borwein polynomial"). Many further applications are discussed.

3.1 Introduction

It was in 1993 at a workshop at Cornell University, when what became known as *the Borwein Conjecture* was born. (One of the authors was an intrigued witness of this event.) George Andrews delivered a two-part lecture on *"AXIOM and the Borwein Conjecture"*, in which he

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— first of all — stated three conjectures that had been communicated to him by Peter Borwein (the first of which became known as "the Borwein Conjecture"), and then reported the lines of attack that he had tried, all of which had failed to give a proof, stressing (quoting from [And95], which contains Andrews' findings in printed form) that *"this is the sort of intriguing simply stated problem that devotees of the theory of partitions love."* Indeed, the statement of the first conjecture, dubbed the "First Borwein Conjecture" in [And95], is the following.

Conjecture 3.1.1 (P. BORWEIN) For all positive integers n, the sign pattern of the coefficients in the expansion of the polynomial $P_n(q)$ defined by

$$P_n(q) := (1-q)(1-q^2)(1-q^4)(1-q^5)\cdots(1-q^{3n-2})(1-q^{3n-1}) \tag{3.1}$$

is $+--+--+--\cdots$, with a coefficient 0 being considered as both $+$ and $-$.

The *Second Borwein Conjecture* from [And95] predicts the same sign behaviour of the coefficients for the square of the "Borwein polynomial".

Conjecture 3.1.2 (P. BORWEIN) For all positive integers n, the sign pattern of the coefficients in the expansion of the polynomial $P_n^2(q)$, where $P_n(q)$ is defined by ((3.1)), is $+--+--+--\cdots$, with the same convention concerning zero coefficients.

The *Third Borwein Conjecture* from [And95] is an assertion on the sign behaviour of the coefficients of a polynomial similar to $P_n(q)$, where however the involved modulus is 5 instead of 3. We shall return to it at the end of this paper, see Conjecture 3.11.1 in Section 3.11.

Interestingly, the first author observed recently that a cubic version of the conjecture also appears to hold, which both Borwein and Andrews missed.

Conjecture 3.1.3 (C. WANG) For all positive integers n, the sign pattern of the coefficients in the expansion of the polynomial $P_n^3(q)$, where $P_n(q)$ is defined by ((3.1)), is $+--+--+--\cdots$, with the same convention concerning zero coefficients as before.

These deceivingly simple conjectures intrigued many researchers after Andrews had introduced them to a larger audience — in particular the first one, Conjecture 3.1.1. Various approaches were tried — combinatorial, or using q-series techniques (cf. e.g. [And95; Ber20b; BW05; Bre96; IKS99; SZ21; War01; War03; Zah06]) —, variations and generalisations were proposed (see [BS19; Bre96; IKS99; SZ21]) — most notably Bressoud's conjecture in [Bre96] — sometimes leading to proofs of related results. However, none of these attempts came anything close to progress concerning the original First Borwein Conjecture, Conjecture 3.1.1. It took almost 30 years until the first author succeeded in proving this conjecture in [Wan22], using analytic means.

Starting point of the proof in [Wan22] was explicit sum representations of the polynomials $A_n(q), B_n(q), C_n(q)$ in the decomposition of $P_n(q)$ given by

$$P_n(q) = A_n(q^3) - qB_n(q^3) - q^2C_n(q^3), \tag{3.2}$$

due to Andrews [And95]. It should be noted that the First Borwein Conjecture, Conjecture 3.1.1, is equivalent to the statement that all coefficients of the polynomials $A_n(q), B_n(q), C_n(q)$ are non-negative. These coefficients were written in [Wan22] in terms of the obvious Cauchy integrals. Subsequent saddle point approximations showed that for $n > 7000$ the coefficient of q^m in $A_n(q), B_n(q), C_n(q)$ is positive in the range $n < m < n^2 - n$. The proof could then be completed by appealing to another result of Andrews [And95] which gives non-negativity of

the coefficients of q^m in $A_n(q), B_n(q), C_n(q)$ for $m \leqslant n$ and $m \geqslant n^2 - n$ "for free", and by performing a computer check of the conjecture for $n \leqslant 7000$.

At this point, it must be mentioned that formulae analogous to Andrews' formulae for the decomposition polynomials $A_n(q), B_n(q), C_n(q)$ are not available for the analogous decompositions of $P_n^2(q)$ or $P_n^3(q)$, or for the corresponding decomposition of the polynomial $S_n(q)$ in the Third Borwein Conjecture (Conjecture 3.11.1), and that it is unlikely that such formulae exist.

Thus, the article [Wan22] left open the question whether it was just an isolated instance that this approach succeeded to prove the First Borwein Conjecture, or whether similar ideas could also lead to proofs of the Second and Third Borwein Conjecture, or of the new Conjecture 3.1.3. Admittedly, since the proof in [Wan22] relied on Andrews' sum representations for the decomposition polynomials $A_n(q), B_n(q), C_n(q)$ in an essential way, at the time it did not seem very realistic to expect that, with these ideas, one could go beyond the First Borwein Conjecture.

In the meantime, however, we realised that, instead of relying on Andrews' sum representations for the decomposition polynomials, the saddle point approximation idea could be directly applied to $P_n(q)$ and its powers, and, when doing this, surprisingly the quantities that have to be approximated are very similar to those that were at stake in [Wan22] (compare, for instance, the sum over m at the beginning of the proof of Proposition 11.1 in [Wan22] with ((3.50)) below, or [Wan22, Lemma B.3] and Lemma 3.A.10). There is a price to pay though: while in [Wan22] the (dominant) saddle points were located on the real axis, with this new approach we have to deal with (dominant) saddle points located at complex points. This makes the estimations that have to be performed more delicate.[2] On the positive side, it allows one to proceed in a more streamlined fashion — for example, here we do not have to deal with several different kinds of peaks along the integration contour, as opposed to [Wan22] where an unbounded number of peaks of two different kinds had to be considered; here we encounter only two peaks that are (complex) conjugate to each other. Most importantly, it allows us to provide a *uniform* proof of the First *and* Second Borwein Conjecture, *as well as* a partial proof of the cubic conjecture, and altogether this is not longer than the proof of "just" the First Borwein Conjecture in [Wan22].

In the next section, we provide an outline of our proof of Conjectures 3.1.1 and 3.1.2, and of "two thirds" of Conjecture 3.1.3. Very roughly, the approach that we put forward consists of the following steps:

1. show that the conjectures hold for the "first few" and the "last few" coefficients (see Part A in Section 3.2);
2. represent the coefficients by a contour integral (see Part B in Section 3.2);
3. divide the contour into two parts, the "peak part" (the part close to the dominant saddle points of the integrand) and the remaining part, the "tail part" (see Part C in Section 3.2);
4. for "large" n (where "large" is made precise), bound the error made by approximating the "peak part" by a Gaußian integral (the "peak error") (see Part D in Section 3.2);
5. for "large" n, bound the error contributed by the "tail part" (the "tail error") (see Part D in Section 3.2);

[2] There is in fact a further subtlety not present in [Wan22] that makes the task of carrying through this new approach more difficult, see Footnotes 3 and 7.

6. verify the conjectures for "small" n (see Part E in Section 3.2);
7. put everything together to complete the proofs (see Part E in Section 3.2).

The details are then filled in in the subsequent sections. More precisely, in Section 3.3 we explain how prior results of Andrews, of Kane, and of Borwein, Borwein and Garvan confirm the conjectures for the "first few" and the "last few" coefficients. Section 3.4 prepares some notation and preliminary material on log-derivatives of the "Borwein polynomial" $P_n(q)$ that is used ubiquitously in the subsequent sections. In Section 3.5, we make our choice of contour for the integral representation precise: it is a circle whose radius satisfies an equation, namely ((3.19)), that approximates the actual saddle point equation. Lemma 3.5.1 presents fundamental properties that this choice satisfies. In Section 3.6, we make precise how we divide the contour into the "peak part" and the "tail part". Lemma 3.6.1 in that section presents first properties of this cutoff, to be used in the later parts of the paper. The fundamental inequality that is derived from this subdivision of the integral contour is the subject of Section 3.7. Namely, Lemma 3.7.1 provides a qualitative upper bound for the resulting approximation of the coefficients of $P_n^\delta(q)$, with $\delta \in \{1, 2, 3\}$, in terms of a peak error term and a tail error term. How to bound the peak error efficiently from above is shown in Section 3.8. This section contains in particular a fundamental result on the approximation of a (complex) function by a Gaußian integral that may be of independent interest for other applications; see Lemma 3.8.1. Subsequently, Section 3.9 is devoted to bound the tail error from above. Finally, in Section 3.10 we put everything together and complete the proofs of Conjectures 3.1.1 and 3.1.2, and of "two thirds" of Conjecture 3.1.3.

Without any doubt, several of the arguments that we need are quite technical. In the interest of not losing pace (too much) while guiding the reader through our proofs, we have "outsourced" some of the auxiliary results and have collected them in an appendix.

It must be emphasised though that a certain "level of technicality" is unavoidable since the approximations that we are carrying out here go with an intrinsic subtlety (already present in [Wan22]) that is absent in most applications of the saddle point approximation technique: our goal is to show that the coefficients of q^m in the "Borwein polynomial" $P_n(q)$ (respectively in its powers) obey a certain sign pattern, with m running through a range that includes the asymptotic orders $O(n^\omega)$, where $1 \leqslant \omega \leqslant 2$. Consequently, our estimations must hold for that entire range, which makes it necessary to manage expressions that contain the radius r of our contour that is solution of the approximate saddle point equation ((3.19)) without further specification of its asymptotic order, as for example in the definition of the cutoff in ((3.25)). The "best" that we can say about r is its range as given in Lemma 3.5.1 (which again — necessarily — covers several different asymptotic orders in terms of n at logarithmic scale).

The last section, Section 3.11, is devoted to a discussion of our approach and further applications. We start by explaining what is missing for the completion of the proof of Conjecture 3.1.3. We discuss the applicability of our methods for proving the Third Borwein Conjecture (see Conjecture 3.11.1), a conjecture of Ismail, Kim and Stanton vastly generalising the First Borwein Conjecture (see Conjecture 3.11.2), or related or similar conjectures, including some new ones that we present in this last section (in particular Conjectures 3.11.3 and 3.11.4). We also point out that the Bressoud Conjecture might as well be amenable to the ideas developed in this paper. Finally, we contemplate on the question whether the Borwein Conjecture(s) should be considered as combinatorial or analytic, a question which is evidently raised by our proof(s) (and other observations).

3.2 An outline of the proof

Here, we provide a brief outline of our proof of Conjectures 3.1.1 and 3.1.2, and of a part of Conjecture 3.1.3. From here on, we use the standard notation for q-shifted factorials,

$$\begin{aligned}(\alpha;q)_n &= (1-\alpha)(1-\alpha q)\cdots(1-\alpha q^{n-1}), \text{ for } n \geqslant 1,\\ (\alpha;q)_0 &= 1.\end{aligned}$$

If $|q| < 1$, or in the sense of formal power series in q, this definition also makes sense for $n = \infty$. Using this notation, the "Borwein polynomial" can be written as

$$P_n(q) = \frac{(q;q)_{3n}}{(q^3;q^3)_n}.$$

Furthermore, in the following we shall write $[q^m]P(q)$ for the coefficient of q^m in the polynomial $P(q)$.

Our goal is to show that the sign pattern of the coefficients

$$[q^m]P_n^\delta(q), \quad m = 0, 1, 2, \ldots,$$

is $+--+--+--\cdots$, where δ is 1, 2, or 3.

Our proof is composed of several parts.

A. THE CONJECTURES HOLD FOR THE "FIRST" $3n+1$ COEFFICIENTS AND THE "LAST" $3n+1$ COEFFICIENTS. We observe that the first few coefficients of $P_n^\delta(q)$ and $P_\infty^\delta(q)$, with $\delta \in \{1,2,3\}$, are identical. More precisely, we have

$$[q^m]P_n^\delta(q) = [q^m]P_\infty^\delta(q) \tag{3.3}$$

for $0 \leqslant m \leqslant 3n$ and $\delta \in \{1,2,3\}$ (actually for all integers δ). By a result of Andrews [And95] this implies the sign pattern of the first $3n+1$ coefficients of $P_n(q)$ as predicted by Conjecture 3.1.1. Similarly, by a result of Kane [Kan04], this implies the sign pattern of the first $3n+1$ coefficients of $P_n^2(q)$ as predicted by Conjecture 3.1.2. By using a result of Borwein, Borwein and Garvan [BBG94], this also implies the sign pattern of the first $3n+1$ coefficients of $P_n^3(q)$ as predicted by Conjecture 3.1.3. See Section 3.3 for the details.

Combining the above observation with the fact that $P_n(q)$, and hence $P_n^\delta(q)$ for all δ, is palindromic, it remains to show that the coefficients of q^m in $P_n^\delta(q)$ for $3n \leqslant m \leqslant (\delta \deg P_n)/2$ follow the sign pattern predicted by Conjectures 3.1.1–3.1.3.

B. CONTOUR INTEGRAL REPRESENTATION OF THE COEFFICIENTS OF $P_n^\delta(q)$. From now on, for convenience, we shall often use $Q_n(q)$ to denote $P_n^\delta(q)$, where δ is 1, 2, or 3.

Using Cauchy's integral formula, the coefficient $[q^m]Q_n(q)$ can be represented as the integral

$$\frac{1}{2\pi i}\int_\Gamma Q_n(q)\frac{dq}{q^{m+1}},$$

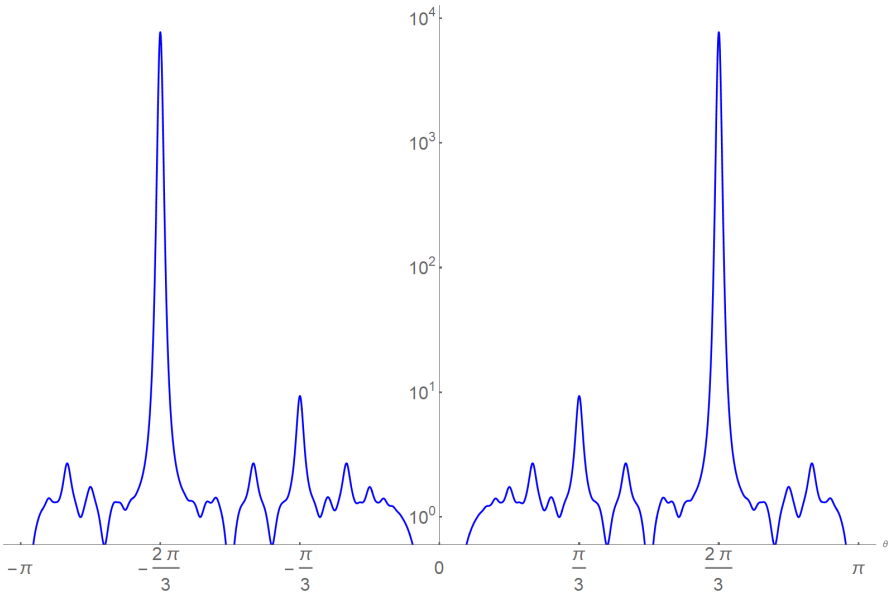

FIGURE 3.1: Modulus of $P_{81}(0.95e^{i\theta})$. The vertical axis has logarithmic scale.

where Γ is any contour about 0 with winding number 1. We will choose Γ as a circle centred at 0 with radius r for some $r \in \mathbb{R}^+$, so that the integral becomes

$$[q^m]Q_n(q) = \frac{r^{-m}}{2\pi} \int_{-\pi}^{\pi} Q_n\left(re^{i\theta}\right) e^{-im\theta}\, d\theta. \tag{3.4}$$

C. THE SADDLE POINT APPROXIMATION. The exact choice of r is related to the *saddle points* of $q \mapsto |q^{-m}Q_n(q)|$, and we will elaborate on this in Section 3.5. The appropriate choice for r is a value smaller than 1 but close to 1, see Lemma 3.5.1.

Figure 3.1 illustrates the typical behaviour of $\theta \mapsto |P_n\left(re^{i\theta}\right)|$ on the circle $\{z \in \mathbb{C} : |z| = r\}$. In particular, we can observe the following general features in the graph:

- the function has two peaks close to $\theta = 2\pi/3$ and $\theta = -2\pi/3$;[3]
- the function values outside small neighbourhoods of $\theta = 2\pi/3$ and $\theta = -2\pi/3$ are very small compared to the peak value.

Based on these heuristics, we choose a cutoff θ_0 (to be determined in ((3.25)) in Section 3.6), and distinguish the following parts of the interval $[-\pi, \pi]$:

- The *peak part* $I_{\text{peak}} := [-2\pi/3 - \theta_0, -2\pi/3 + \theta_0] \cup [2\pi/3 - \theta_0, 2\pi/3 + \theta_0]$.
- The *tail part* $I_{\text{tail}} := [-\pi, \pi] \backslash I_{\text{peak}}$.

Naturally, the integral ((3.4)) can be divided into two subintegrals corresponding to the two parts above.

[3]The actual locations of the peaks have arguments slightly off $\theta = \pm 2\pi/3$. This is one of the delicate points of the estimations to be performed.

We make the following observations concerning the subintegrals:

• The subintegral $\int_{I_{\text{peak}}} Q_n\left(re^{i\theta}\right) e^{-im\theta}\, d\theta$ can be approximated by a Gaußian integral. More specifically, if we define

$$g_{Q_n}(r) = -\operatorname{Re}\frac{\partial^2}{\partial\theta^2}\log Q_n(re^{i\theta})\Big|_{\theta=2\pi/3}, \tag{3.5}$$

then we have

$$\begin{aligned}\int_{2\pi/3-\theta_0}^{2\pi/3+\theta_0} Q_n(re^{i\theta})e^{-im\theta}\, d\theta &= e^{-2\pi mi/3}\int_{-\theta_0}^{\theta_0} Q_n(re^{i(\theta+2\pi/3)})e^{-im\theta}\, d\theta \\ &\approx e^{-2\pi mi/3}Q_n(re^{2\pi i/3})\int_{-\theta_0}^{\theta_0} e^{-g_{Q_n}(r)\theta^2/2}\, d\theta \\ &= e^{-2\pi mi/3}Q_n(re^{2\pi i/3})\frac{\sqrt{2\pi}}{\sqrt{g_{Q_n}(r)}}\operatorname{erf}\left(\frac{\theta_0\sqrt{g_{Q_n}(r)}}{\sqrt{2}}\right).\end{aligned} \tag{3.6}$$

Here, "≈" means "approximated by". Since $Q_n(q)$ is a polynomial with real coefficients, we have $Q_n(\bar{z}) = \overline{Q_n(z)}$. Therefore, an analogous approximation holds for the other interval of I_{peak}, that is, for the integral over θ in $[-2\pi/3-\theta_0, -2\pi/3+\theta_0]$. The error made by these approximations is captured by the term $\epsilon_{0,Q_n}(m,r)$ defined below.

• The subintegral over I_{tail} can be bounded above by

$$\left|\int_{I_{\text{tail}}} Q_n(re^{i\theta})e^{-im\theta}\, d\theta\right| \leqslant \left|Q_n(re^{2\pi i/3})\right|\int_{I_{\text{tail}}}\left|\frac{Q_n(re^{i\theta})}{Q_n(re^{2\pi i/3})}\right| d\theta. \tag{3.7}$$

The error of this approximation is captured by the term $\epsilon_{1,Q_n}(r)$ defined below.

D. Bounding the errors. Our next step is to estimate the error in the approximation ((3.6)) of the peak part, and to bound the tail part ((3.7)) of the integral. Accordingly, we define the error terms $\epsilon_{0,Q_n}(m,r)$ and $\epsilon_{1,Q_n}(r)$. Both are *relative* errors, namely relative to the modulus of the (presumably, at this point) dominating part

$$|Q_n(re^{2\pi i/3})|\frac{\sqrt{2\pi}}{\sqrt{g_{Q_n}(r)}}\operatorname{erf}\left(\frac{\theta_0\sqrt{g_{Q_n}(r)}}{\sqrt{2}}\right)$$

(cf. ((3.6))). Namely, we define

$$\begin{aligned}&\epsilon_{0,Q_n}(m,r) \\ &:= 2\left|\frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\operatorname{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\int_{-\theta_0}^{\theta_0}\left(\frac{Q_n(re^{i(\theta+2\pi/3)})}{Q_n(re^{2\pi i/3})}e^{-im\theta} - e^{-g_{Q_n}(r)\theta^2/2}\right) d\theta\right|\end{aligned} \tag{3.8}$$

and

$$\epsilon_{1,Q_n}(r) := \frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\operatorname{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\int_{I_{\text{tail}}}\left|\frac{Q_n(re^{i\theta})}{Q_n(re^{2\pi i/3})}\right| d\theta. \tag{3.9}$$

In Lemma 3.7.1 in Section 3.7, we show that, with these error terms, the coefficient of q^m in $Q_n(q)$ can be approximated by

$$\left|\frac{r^m\sqrt{2\pi g_{Q_n}(r)}}{\operatorname{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\frac{1}{|Q_n(re^{2\pi i/3})|}[q^m]Q_n(q) - 2\cos\left(\arg Q_n(re^{2\pi i/3}) - 2m\pi/3\right)\right| \leqslant \epsilon_{0,Q_n}(m,r) + \epsilon_{1,Q_n}(r). \quad (3.10)$$

Therefore, there are two things to accomplish, the second required by the first:

1. Show that the error terms $\epsilon_{0,Q_n}(m,r)$ and $\epsilon_{1,Q_n}(r)$ are small enough to satisfy the inequality
$$\epsilon_{0,Q_n}(m,r) + \epsilon_{1,Q_n}(r) < \left|2\cos\left(\arg Q_n(re^{2\pi i/3}) - 2m\pi/3\right)\right|. \quad (3.11)$$
2. Get a control on $\arg Q_n(re^{2\pi i/3})$ and show that it is less than $\frac{2\pi}{3} - \frac{\pi}{2} = \frac{\pi}{6}$ in absolute value.

Both together allow us to conclude that $[q^m]Q_n(q)$ has the same sign as the cosine term on the right-hand side of ((3.11)), that is, it is positive if $m \equiv 0 \pmod 3$ and negative otherwise, exactly as predicted by Conjectures 3.1.1–3.1.3.

The peak error $\epsilon_{0,Q_n}(m,r)$ is estimated in Section 3.8 (see Lemma 3.8.3), and Section 3.9 treats the tail error $\epsilon_{1,Q_n}(r)$ (see Lemma 3.9.4).

E. Concluding the proof. As explained in the preceding Part D, the tasks formulated in Items (1) and (2) above must be accomplished. Task (2) is taken care of in Lemma 3.10.1. By combining this with the obtained bounds on $\epsilon_{0,Q_n}(m,r)$ and $\epsilon_{1,Q_n}(r)$, Task (1) is carried out in the remaining parts of Section 3.10 for "large" n. In combination with suitable direct calculations for "small" n, this leads to full proofs of the First and Second Borwein Conjecture, and to a partial proof of the Cubic Borwein Conjecture, see Theorems 3.10.2, 3.10.3 and 3.10.4.

3.3 The infinite cases

In this section, we show that the first $3n+1$ coefficients of $P_n^\delta(q)$, where δ is 1, 2, or 3, follow the sign pattern $+--+--+--\cdots$, by using the simple fact, observed before in ((3.3)), that they agree with the corresponding coefficients of $P_\infty^\delta(q)$, and by exploiting known properties of the expansions of $P_\infty^\delta(q)$.

Andrews [And95, Eqs. (4.2)–(4.4)] showed that

$$P_\infty(q) = \frac{(q;q)_\infty}{(q^3;q^3)_\infty} = \frac{(q^{12},q^{15},q^{27};q^{27})_\infty - q(q^6,q^{21},q^{27};q^{27})_\infty - q^2(q^3,q^{24},q^{27};q^{27})_\infty}{(q^3;q^3)_\infty}.$$

Clearly, this implies that the sign pattern of the coefficients of $P_\infty(q)$ is $+--+--+--\cdots$.[4]

[4]We point out that this sign pattern of the coefficients of $P_\infty(q)$ also follows from a general result of Andrews [And95, Theorem 2.1] that, according to [And95], has also been independently obtained by Garvan and P. Borwein.

Using the circle method, Kane [Kan04] established the sign pattern $+--+--+--\cdots$ for the power series $(q;q)_\infty^2/(q^3;q^3)_\infty$, except for the coefficient of q^5 which is equal to 1. A multiplication with the series $(q^3;q^3)_\infty^{-1}$ (which has positive coefficients) transforms this power series into $P_\infty^2(q)$, and in the process removes the mentioned outlier.

Finally, it follows from results of Borwein, Borwein and Garvan [BBG94] that

$$\frac{(q;q)_\infty^3}{(q^3;q^3)_\infty} = \sum_{m,n\in\mathbb{Z}} q^{3(m^2+mn+n^2)} - q\sum_{m,n\in\mathbb{Z}} q^{3(m^2+mn+n^2+m+n)}, \tag{3.12}$$

where, as usual, $\mathbb{Z}$ denotes the set of integers. To be precise, from Items (ii) and (iii) of Lemma 2.1 in [BBG94], one can derive the equation $b(q) = a(q^3) - c(q^3)$. Proposition 2.2 in [BBG94] shows that $b(q)$ equals the left-hand side in ((3.12)), while the definitions of $a(q^3)$ and $b(q^3)$ from [BBG94] are as stated on the right-hand side of ((3.12)). As before, multiplication of both sides of ((3.12)) by $(q^3;q^3)_\infty^{-2}$, which is a power series with non-negative coefficients, shows that the coefficients of $P_n^3(q)$ follow the sign pattern $+--+--+--\cdot$.[5]

It should be noted however that ((3.12)) also implies that the coefficients of q^{3m+2} in $P_\infty^3(q)$ are zero for all m. This observation, and its implications, will be discussed in more detail in Item (1) of Section 3.11.

3.4 The log-derivatives of the "Borwein polynomial" $P_n(q)$

In this section, we present some basic facts on derivatives of $\log P_n(re^{i\theta})$ with respect to θ. These will be used ubiquitously in the subsequent sections.

By routine calculation, we see that the j-th derivative of $\log P_n(re^{i\theta})$, "centred" at $\theta = 2\pi/3$, can be expressed as

$$\left(\frac{\partial}{\partial\theta}\right)^j \log P_n(re^{i\theta}) = \frac{1}{2}i^j U_j(n, re^{i(\theta-2\pi/3)}) + \frac{\sqrt{3}}{2}i^{j-1}V_j(n, re^{i(\theta-2\pi/3)}), \tag{3.13}$$

where

$$U_j(n,z) := \sum_{k=1}^{n}\left((3k-2)^j u_j(z^{3k-2}) + (3k-1)^j u_j(z^{3k-1})\right), \tag{3.14}$$

$$V_j(n,z) := \sum_{k=1}^{n}\left((3k-2)^j v_j(z^{3k-2}) - (3k-1)^j v_j(z^{3k-1})\right), \tag{3.15}$$

and the rational functions u_j and v_j are given by

$$u_j(z) := \left(z\frac{d}{dz}\right)^{j-1}\frac{z(1+2z)}{1+z+z^2}, \tag{3.16}$$

$$v_j(z) := \left(z\frac{d}{dz}\right)^{j-1}\frac{z}{1+z+z^2}. \tag{3.17}$$

[5] We point out that this sign pattern of the coefficients of $P_\infty^3(q)$ also follows from a general result of Schlosser and Zhou [SZ21, Theorem 6].

In particular, the first few of these functions are given by

$$\begin{aligned}
u_1(z) &= \frac{z(1+2z)}{1+z+z^2},\\
v_1(z) &= \frac{z}{1+z+z^2},\\
u_2(z) &= \frac{z(1+4z+z^2)}{(1+z+z^2)^2},\\
v_2(z) &= \frac{z(1-z^2)}{(1+z+z^2)^2},\\
u_3(z) &= \frac{z(1-z^2)(1+7z+z^2)}{(1+z+z^2)^3},\\
v_3(z) &= \frac{z(1-z-6z^2-z^3+z^4)}{(1+z+z^2)^3},\\
u_4(z) &= \frac{z(1+12z-12z^2-56z^3-12z^4+12z^5+z^6)}{(1+z+z^2)^4},\\
v_4(z) &= \frac{z(1-z^2)(1-4z-21z^2-4z^3+z^4)}{(1+z+z^2)^4}.
\end{aligned}$$

We also define the sums

$$X_j(n,r) := \sum_{\substack{k=1\\3\nmid k}}^{3n} k^j r^k = \sum_{k=1}^{3n} k^j r^k - 3^j \sum_{k=1}^{n} k^j (r^3)^k, \tag{3.18}$$

and denote the corresponding infinite sum by $X_j(\infty, r)$. It is easy to see that $(1-r^3)^{j+1}X_j(n,r)$ is a polynomial in n, r and r^n. Furthermore, $X_j(n,r)$ is increasing with respect to both n and r. A collection of inequalities between various products of these sums is given in Lemma 3.A.7. These inequalities are used in the estimations in Section 3.8.

3.5 Locating the dominant (approximate) saddle points

The results of Section 3.3, and the fact that the polynomial $P_n(q)$ is palindromic for all n, together show that it suffices to consider $[q^m]Q_n(q)$ for $m \in [3n, (\deg Q_n)/2]$, where Q_n is chosen as $P_n^\delta(q)$ for $\delta \in \{1,2,3\}$, as before. The purpose of this section is to describe our choice of the radius r in ((3.4)).

Ideally, in line with standard practice in analytic combinatorics, the radius r in the integral in ((3.4)) should be chosen such that the circle $\theta \mapsto re^{i\theta}$, $-\pi \leqslant \theta \leqslant \pi$, passes through the dominant saddle point(s)[6] of the function $q \mapsto |q^{-m}Q_n(q)|$. If $Q_n(q)$ has non-negative coefficients, according to Pringsheim's theorem, the dominant saddle point is located on the positive real axis, and the problem is equivalent to the minimisation of the quantity $r^{-m}Q_n(r)$.

[6]Here, "dominant saddle point(s)" means "the saddle point(s) with largest modulus of the integrand". We shall sometimes also abuse terminology and speak of "dominant peaks".

In our case however, the dominant saddle points are located near the complex third roots of unity instead of on the positive real axis. In analogy to the process above, we choose the radius r so that the quantity $r^{-m}\left|Q_n(re^{2\pi i/3})\right|$ is minimised. By taking a log-derivative, and substituting $Q_n = P_n^{\delta}(q)$, we obtain an equation in terms of r:[7]

$$r\,\mathrm{Re}\left(\frac{d}{dr}\log P_n(re^{2\pi i/3})\right) = \frac{m}{\delta}. \tag{3.19}$$

It must be emphasised that the solution r of this equation (it will indeed be shown in Lemma 3.5.1 below that there is a unique solution) depends on n and m (and δ of course). We will however most of the time suppress this dependency in the interest of better readability. Only occasionally, when we think that this is necessary, we will add an index that indicates the dependency (as for example in Lemmas 3.5.1 and 3.8.3, or in the proofs of Theorems 3.10.2, 3.10.3 and 3.10.4).

It turns out that, under the above restriction on m, the minimiser radius r approaches 1 as $n \to \infty$. These observations are proved in the following lemma. They are crucial in our estimations of the error terms ϵ_{i,Q_n}, $i = 0, 1$.

Lemma 3.5.1 *For all integers $n \geqslant 1$ and $m \in (0, \delta \deg P_n)$, with $\delta \in \{1, 2, 3\}$, the approximate saddle point equation ((3.19)) has a unique solution $r = r_{m,n} \in \mathbb{R}^+$. Moreover, if $3n \leqslant m \leqslant (\delta \deg P_n)/2$, then we have $r_0 < r \leqslant 1$, where*

$$r_0 = e^{-\sqrt{4\delta/27n}}. \tag{3.20}$$

Furthermore, as a function in m, the solution $r = r_{m,n}$ to ((3.19)) is increasing.

Proof: We infer from ((3.13)) that the left-hand side of ((3.19)) can be written as

$$r\,\mathrm{Re}\left(\frac{d}{dr}\log P_n(re^{2\pi i/3})\right) = \frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3n} k u_1(r^k), \tag{3.21}$$

where $u_1(x) = x(1+2x)/(1+x+x^2)$ is defined as in Section 3.4.

Therefore, Equation ((3.19)) is equivalent to

$$\sum_{\substack{k=1\\3\nmid k}}^{3n} k u_1(r^k) = \frac{2m}{\delta}. \tag{3.22}$$

Note that

$$u_1'(r) = \frac{1+4r+r^2}{(1+r+r^2)^2} > 0, \tag{3.23}$$

[7] The reader must be warned: this is *not* the saddle point equation! The saddle point equation is $q\frac{d}{dq}P_n(q) = m/\delta$, as an equation for complex q. It will have two solutions with arguments *close* to $\pm 2\pi/3$, but not *exactly* $\pm 2\pi/3$. Equation ((3.19)) is a "saddle point-like equation", in which the argument of the solution is "frozen" to $2\pi/3$. In our analysis, it mimics the role of a saddle point equation, but is in fact "just" an "approximate" saddle point equation. We made this deliberate choice since we deemed it unfeasible to carry through the programme of approximations without having a firm control on the arguments of the (approximate or not) saddle points. As it turns out, this is nevertheless good enough for performing our estimations.

so u_1 is increasing. Moreover, we have the special values

$$u_1(0) = 0, \qquad u_1(1) = 1, \qquad \lim_{r\to+\infty} u_1(r) = 2. \tag{3.24}$$

Along with the fact that

$$\deg P_n = \sum_{\substack{k=1\\3\nmid k}}^{3n} k,$$

these special values imply that the sum

$$\sum_{\substack{k=1\\3\nmid k}}^{3n} k u_1(r^k)/2$$

tends to 0, $(\deg P_n)/2$, and $\deg P_n$ when $r \to 0, 1, +\infty$, respectively. The existence and uniqueness of solution, as well as the upper bound $r \leqslant 1$, follow from the intermediate value theorem.

It remains to prove the lower bound on r. Since u_1 is increasing, it suffices to show that

$$\sum_{\substack{k=1\\3\nmid k}}^{3n} k u_1(r_0^k) < \frac{6n}{\delta}.$$

Equation ((3.88)) in Lemma 3.A.1 implies that

$$\begin{aligned}\sum_{\substack{k=1\\3\nmid k}}^{3n} k u_1(r_0^k) &< \frac{2}{\sqrt{3}} \sum_{\substack{k=1\\3\nmid k}}^{3n} k r_0^k < \frac{2}{\sqrt{3}} \sum_{\substack{k=1\\3\nmid k}}^{\infty} k r_0^k \\ &= \frac{2}{\sqrt{3}} \frac{r_0(1 + 2r_0 + 2r_0^3 + r_0^4)}{(1 - r_0^3)^2} < \frac{8}{9}(-\log r_0)^{-2} = \frac{6n}{\delta},\end{aligned}$$

where the last inequality used the fact that the maximum of the function

$$r \mapsto \frac{2r(1 + 2r + 2r^3 + r^4)(-\log r)^2}{\sqrt{3}(1 - r^3)^2}$$

on $[0, 1]$ is approximately $0.881906 < 8/9$.

For the additional assertion at the end of the lemma, we recall from ((3.23)) that $u_1(r)$ is increasing in r. Therefore, by ((3.22)), if m is increasing, so must be r. □

3.6 The choice of cutoff

Our choice of the cutoff θ_0 announced in Part C of Section 3.2 is

$$\theta_0 := C_0 \frac{1 - r^3}{1 - r^{3n}}, \tag{3.25}$$

where the constant C_0 is chosen as $\frac{10}{81}$.

We give some immediate consequences of ((3.20)) and ((3.25)), to be used in the following two sections.

Lemma 3.6.1 *With $\mathbb{Z}^+$ denoting the set of positive integers, suppose that $n \in \mathbb{Z}^+$, $\delta \in \{1, 2, 3\}$, $t \geqslant 0$, and r_0 and θ_0 are defined as in ((3.20)) and ((3.25)), respectively. Then the following results hold for $r \in (r_0, 1]$ and $\theta \in [-t\theta_0, t\theta_0]$:*

1. *For $n \geqslant 4$, we have*
$$\frac{1 - r_0^3}{1 - r_0^{3n}} \leqslant -3 \log r_0, \tag{3.26}$$
and consequently
$$\left|\log re^{i\theta}\right| < (1 + 3tC_0)(-\log r_0) \leqslant \frac{2(1 + 3tC_0)}{3\sqrt{n}}. \tag{3.27}$$

2. *For $k \in [0, 3n]$, the complex number $r^k e^{ik\theta}$ belongs to the region S_{3tC_0}, where S_ρ is defined by*
$$S_\rho := \left\{ Re^{i\Theta} : 0 \leqslant R \leqslant 1 \text{ and } |\Theta| \leqslant \rho \frac{-\log R}{1 - R} \right\} \tag{3.28}$$
for $\rho > 0$.

3. *Suppose $|\theta| \leqslant t\theta_0$ for some $t \geqslant 0$. For $r \in (r_0, 1]$ and $\ell \in \mathbb{Z}^+$, we have*
$$\sup_{k \in [0,3n]} \left|\log re^{i\theta}\right|^\ell k^\ell r^k \leqslant \ell^\ell (e^{-1} + 3tC_0)^\ell. \tag{3.29}$$

4. *For $j \geqslant 0$, let $X_j(n, r)$ be defined as in ((3.18)). Then, for $n \geqslant 400$ and $r \in (r_0, 1]$, we have*
$$X_0(n, r) > 0.95\sqrt{n}, \tag{3.30}$$
$$X_1(n, r) > 1.35n, \tag{3.31}$$
$$X_3(n, r) > 16n^2, \tag{3.32}$$
$$X_4(n, r) > 94n^{5/2}. \tag{3.33}$$

Proof: (1) We have $-\log r_0 = \sqrt{4\delta/27n} \leqslant \sqrt{12/108} = 1/3$. Next we substitute $x := -3 \log r_0$ in the inequality $(1 - e^{-x})/x \leqslant 1 - e^{-1/x}$ (valid for $0 \leqslant x \leqslant 1$) to obtain

$$\frac{1 - r_0^3}{-3 \log r_0} \leqslant 1 - e^{\frac{1}{3 \log r_0}} < 1 - e^{3n \log r_0} = 1 - r_0^{3n},$$

where the last inequality holds because $9n(\log r_0)^2 = 4\delta/3 > 1$. The inequality ((3.27)) follows from

$$\left|\log re^{i\theta}\right| \leqslant -\log r + t\theta_0 \leqslant -\log r_0 + tC_0 \frac{1 - r_0^3}{1 - r_0^{3n}} \leqslant (1 + 3tC_0)(-\log r_0).$$

(2) The definition ((3.25)) implies that

$$k|\theta| \leqslant ktC_0 \frac{1-r^3}{1-r^{3n}} \leqslant ktC_0 \frac{-\log r^3}{1-r^k} = 3tC_0 \frac{-\log r^k}{1-r^k}.$$

(3) We first note that

$$\left(\sup_{k\in[0,3n]} k^\ell r^k\right)^{1/\ell} = \begin{cases} \frac{\ell}{e(-\log r)}, & \text{if } r \leqslant e^{-\ell/(3n)}, \\ 3nr^{3n/\ell}, & \text{if } r > e^{-\ell/(3n)}. \end{cases}$$

On the other hand, we have $\left|\log re^{i\theta}\right| \leqslant -\log r + |\theta| \leqslant -\log r + t\theta_0$, and therefore

$$\begin{aligned}
\left|\log re^{i\theta}\right| \left(\sup_{k\in[0,3n]} k^\ell r^k\right)^{1/\ell} &\leqslant \frac{\ell}{e} + t\theta_0 \begin{cases} \frac{\ell}{e(-\log r)}, & \text{if } r \leqslant e^{-\ell/(3n)}, \\ 3nr^{3n/\ell}, & \text{if } r > e^{-\ell/(3n)}, \end{cases} \\
&= \frac{\ell}{e} + 3\ell tC_0 \begin{cases} \frac{(1-r^3)}{e(-\log r^3)(1-r^{3n})}, & \text{if } r \leqslant e^{-\ell/(3n)}, \\ \frac{n(1-r^3)r^{3n/\ell}}{\ell(1-r^{3n})}, & \text{if } r > e^{-\ell/(3n)}, \end{cases} \\
&\leqslant \frac{\ell}{e} + 3\ell tC_0 \begin{cases} \frac{1}{e(1-e^{-\ell})}, & \text{if } r \leqslant e^{-\ell/(3n)}, \\ \frac{r^{3n/\ell}(-\log r^{3n/\ell})}{1-r^{3n/\ell}}, & \text{if } r > e^{-\ell/(3n)}, \end{cases} \\
&\leqslant \frac{\ell}{e} + 3\ell tC_0 \begin{cases} \frac{1}{e(1-e^{-\ell})}, & \text{if } r \leqslant e^{-\ell/(3n)}, \\ 1, & \text{if } r > e^{-\ell/(3n)}, \end{cases} \\
&\leqslant \frac{\ell}{e} + 3\ell tC_0.
\end{aligned}$$

(4) We first note that, for all j, n and $r \in [0,1]$, we have

$$X_j(\infty, r) - X_j(n, r) = \sum_{\substack{k=1 \\ 3\nmid k}}^{\infty} r^{3n+k}(3n+k)^j < r^{3n} \sum_{\substack{k=1 \\ 3\nmid k}}^{\infty} r^k(3nk+k)^j = r^{3n}(3n+1)^j X_j(\infty, r).$$

Thus,

$$X_j(n, r) > X_j(\infty, r)\left(1 - (3n+1)^j r^{3n}\right).$$

The only place where δ figures in the inequalities ((3.30))–((3.33)) is in r_0, which, in its turn, determines the range for r, namely the interval $(r_0, 1]$. This interval is largest for $\delta = 3$. Clearly, it suffices to consider that case. Hence, from here on we assume that $\delta = 3$ and correspondingly $r_0 = e^{-2/(3\sqrt{n})}$.

By the above considerations, we have

$$\begin{aligned}
X_j(n, r) &> X_j(n, r_0) > X_j(\infty, r_0)\left(1 - (3n+1)^j r_0^{3n}\right) \\
&= X_j(\infty, r_0)\left(1 - (3n+1)^j e^{-2\sqrt{n}}\right) \\
&\geqslant (-3\log r_0)^{-j-1}\left(X_j(\infty, r_0)(1-r_0^3)^{j+1}\right)\left(1 - (3n+1)^j e^{-2\sqrt{n}}\right)
\end{aligned}$$

$$\geqslant n^{(j+1)/2} 2^{-j-1} \left(X_j(\infty, r_0)(1-r_0^3)^{j+1}\right) \left(1-(3n+1)^j e^{-2\sqrt{n}}\right).$$

Since $X_j(\infty, r_0)(1-r_0^3)^{j+1}$ is a polynomial in r_0 with non-negative coefficients (and therefore increasing with respect to n) and $(3n+1)^j e^{-2\sqrt{n}}$ is evidently decreasing with respect to n whenever $n \geqslant j^2$, the inequalities ((3.30))–((3.33)) follow from evaluating the factor

$$2^{-j-1} \left(X_j(\infty, r_0)(1-r_0^3)^{j+1}\right) \left(1-(3n+1)^j e^{-2\sqrt{n}}\right)$$

at $n = 400$ and $j = 0, 1, 3, 4$. □

3.7 The fundamental error inequality

In this section we prove the fundamental inequality, claimed in ((3.10)), that provides an upper bound for the approximation of the coefficient of q^m in $Q_n(q) = P_n^\delta(q)$, where $\delta \in \{1, 2, 3\}$, in terms of the error terms $\epsilon_{0,Q_n}(m, r)$ and $\epsilon_{1,Q_n}(r)$ defined in ((3.8)) and ((3.9)).

Lemma 3.7.1 *With the notations from Section 3.2, we have*

$$\left| \frac{r^m \sqrt{2\pi g_{Q_n}(r)}}{\operatorname{erf}\left(\theta_0 \sqrt{g_{Q_n}(r)/2}\right)} \frac{1}{|Q_n(re^{2\pi i/3})|} [q^m] Q_n(q) - 2\cos\left(\arg Q_n(re^{2\pi i/3}) - 2m\pi/3\right) \right| \leqslant \epsilon_{0,Q_n}(m, r) + \epsilon_{1,Q_n}(r). \quad (3.34)$$

Proof: Denoting the argument of $Q_n(re^{2\pi i/3})$ temporarily by γ, from the integral representation ((3.4)) of the coefficient of q^m in $Q_n(q)$ and the division of the integration interval $[-\pi, \pi]$ into I_{peak} and I_{tail} (see Part C in Section 3.2), we obtain

$$\begin{aligned}
\frac{1}{|Q_n(re^{2\pi i/3})|}[q^m]Q_n(q) &= e^{i\gamma}\frac{r^{-m}}{2\pi}\int_{-\pi}^{\pi}\frac{Q_n\left(re^{i\theta}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta \\
&= e^{i\gamma}\frac{r^{-m}}{2\pi}\left(\int_{2\pi/3-\theta_0}^{2\pi/3+\theta_0}\frac{Q_n\left(re^{i\theta}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta + \int_{-2\pi/3-\theta_0}^{-2\pi/3+\theta_0}\frac{Q_n\left(re^{i\theta}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta \right. \\
&\qquad \left. + \int_{I_{\text{tail}}}\frac{Q_n\left(re^{i\theta}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta\right) \\
&= \frac{r^{-m}}{2\pi}\left(e^{i\gamma-2m\pi i/3}\int_{-\theta_0}^{\theta_0}\frac{Q_n\left(re^{i(\theta+2\pi/3)}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta \right. \\
&\qquad \left. + e^{i\gamma+2m\pi i/3-2i\gamma}\int_{-\theta_0}^{\theta_0}\frac{Q_n\left(re^{i(\theta-2\pi/3)}\right)}{Q_n(re^{-2\pi i/3})}e^{-im\theta}\,d\theta + e^{i\gamma}\int_{I_{\text{tail}}}\frac{Q_n\left(re^{i\theta}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta\right),
\end{aligned}$$

where we used the earlier observed fact that $Q_n(\bar{z}) = \overline{Q_n(z)}$ twice to obtain the last line. Using this relation and the definitions ((3.8)) and ((3.9)) of the error terms, we are led to the following estimation:

$$\left| \frac{r^m \sqrt{2\pi g_{Q_n}(r)}}{\operatorname{erf}\left(\theta_0 \sqrt{g_{Q_n}(r)/2}\right)} \frac{1}{|Q_n(re^{2\pi i/3})|} [q^m] Q_n(q) \right.$$

$$
\begin{aligned}
&\quad - \frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\,\mathrm{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\left(e^{i(\gamma-2m\pi/3)}+e^{-i(\gamma-2m\pi/3)}\right)\int_{-\theta_0}^{\theta_0} e^{-g_{Q_n}(r)\theta^2/2}\,d\theta\Bigg| \\
&\leqslant \left|\frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\,\mathrm{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\int_{-\theta_0}^{\theta_0}\left(\frac{Q_n\left(re^{i(\theta+2\pi/3)}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}-e^{-g_{Q_n}(r)\theta^2/2}\right)d\theta\right| \\
&\quad + \left|\frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\,\mathrm{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\int_{-\theta_0}^{\theta_0}\left(\frac{Q_n\left(re^{i(\theta-2\pi/3)}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}-e^{-g_{Q_n}(r)\theta^2/2}\right)d\theta\right| \\
&\quad + \left|\frac{\sqrt{g_{Q_n}(r)}}{\sqrt{2\pi}\,\mathrm{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)}\int_{I_{\text{tail}}}\frac{Q_n\left(re^{i(\theta+2\pi/3)}\right)}{Q_n(re^{2\pi i/3})}e^{-im\theta}\,d\theta\right| \\
&\leqslant \epsilon_{0,Q_n}(m,r)+\epsilon_{1,Q_n}(r).
\end{aligned}
$$

By the definition of the Gauß error function, this turns out to be equivalent to ((3.34)). □

3.8 Bounding the peak error

The goal of the section is to provide a bound for the peak error term $\epsilon_{0,Q_n}(m,r)=\epsilon_{0,P_n^\delta}(m,r)$ (cf. ((3.8))). We will derive it from a general bound on relative errors for the approximation of a (complex) function by a Gaußian, given in Lemma 3.8.1 below. To serve our purpose, we must apply this lemma to the function in ((3.49)). In order to be able to do this, we have to first provide bounds for the various constants, defined by the derivatives of the function, that appear in the lemma. This is done in Lemma 3.8.2. After these preparations, our bound for $\epsilon_{0,Q_n}(m,r)$ is presented, and proved, in Lemma 3.8.3.

Here is the announced general result about bounding relative errors of the approximation of a (complex) function by a Gaußian from above.

Lemma 3.8.1 *Suppose that $x_0>0$ and $f\in C^4([-x_0,x_0];\mathbb{C})$ with $f(0)=0$. We define $f_k:=f^{(k)}(0)$ for $k=1,2$ as well as*

$$f_3:=3\int_0^1(1-t)^2\sup_{|x|\leqslant tx_0}|f^{(3)}(x)|\,dt$$

and

$$f_4:=4\int_0^1(1-t)^3\sup_{|x|\leqslant tx_0}\left|f^{(4)}(x)\right|\,dt,$$

and we write $g=-\operatorname{Re}f_2$ for simplicity.

Suppose further that $f_1\in\mathbb{R}$, $g>0$, that $\mu_3:=\frac{x_0f_3}{3g}\in(0,1)$, and that $\mu_4:=\frac{x_0\sqrt{f_4}}{\sqrt{8g}}\in(0,1)$. Then we have

$$
\begin{aligned}
&\left|\sqrt{\frac{g}{2\pi}}\int_{-x_0}^{x_0}\left(e^{f(x)}-e^{-gx^2/2}\right)dx\right|\leqslant \mathrm{erf}\left(x_0\sqrt{\frac{g}{2}}\right)\cosh(f_1x_0) \\
&\times\left(\frac{|\operatorname{Im}f_2|+f_1^2}{2g}+\frac{4f_3\beta_1(\mu_3)}{9\sqrt{\pi}g^3}+\frac{f_4\beta_3(\mu_4)}{3\sqrt{\pi}g^2}+\frac{4f_1f_3\beta_2(\mu_3)}{3\sqrt{\pi}g^2}+\frac{\sqrt{2}f_1f_4\beta_4(\mu_4)}{3\sqrt{\pi}g^{5/2}}\right),
\end{aligned}
\tag{3.35}
$$

where the functions β_i, $i = 1, 2, 3, 4$, are as defined in Lemma 3.A.3.
Proof: Let $R_2(x) = f(x) - f_1 x - f_2 x^2/2$ be the second order Taylor remainder term of $f(x)$ at $x = 0$, and let $R_e(x) = (R_2(x) + R_2(-x))/2$. Taylor's theorem (with the remainder in integral form) implies that

$$|R_2(x)| \leqslant \frac{f_3}{6}|x|^3 \quad \text{and} \quad |R_e(x)| \leqslant \frac{f_4}{24}|x|^4. \tag{3.36}$$

We split the function $e^{f(x)} - e^{-gx^2/2}$ as follows:

$$\begin{aligned} e^{f(x)} - e^{-gx^2/2} = e^{-gx^2/2}(e^{f_1 x + i \operatorname{Im} f_2 x^2/2} - 1) \\ + \cosh(f_1 x) e^{f_2 x^2/2}\left(e^{R_2(x)} - 1\right) \\ + \sinh(f_1 x) e^{f_2 x^2/2}\left(e^{R_2(x)} - 1\right). \end{aligned}$$

Subsequently, we consider the integral of each term over $[-x_0, x_0]$.

The integral of the first term is controlled by

$$\begin{aligned} &\left|\int_{-x_0}^{x_0} e^{-gx^2/2}\left(e^{f_1 x + i \operatorname{Im} f_2 x^2/2} - 1\right)\right| dx \\ &\quad = \left|\int_0^{x_0} e^{-gx^2/2}(e^{f_1 x + i \operatorname{Im} f_2 x^2/2} + e^{-f_1 x + i \operatorname{Im} f_2 x^2/2} - 2)\right| dx \\ &\quad \leqslant \int_0^{x_0} e^{-gx^2/2}\left(\left|\left(e^{f_1 x} + e^{-f_1 x}\right)\left(e^{i \operatorname{Im} f_2 x^2/2} - 1\right)\right| + \left|e^{f_1 x} + e^{-f_1 x} - 2\right|\right) dx \\ &\quad \leqslant \int_0^{x_0} e^{-gx^2/2}\left(2\cosh(f_1 x_0)|\operatorname{Im} f_2|\frac{x^2}{2} + \cosh(f_1 x_0) f_1^2 x^2\right) dx \\ &\quad = \cosh(f_1 x_0)\left(|\operatorname{Im} f_2| + f_1^2\right)\int_0^{x_0} x^2 e^{-gx^2/2}\, dx \\ &\quad < \frac{\cosh(f_1 x_0)(|\operatorname{Im} f_2| + f_1^2)}{g}\sqrt{\frac{\pi}{2g}}\operatorname{erf}\left(x_0\sqrt{\frac{g}{2}}\right). \end{aligned}$$

For the second term, we utilise ((3.107)), ((3.36)), ((3.102)) (with $u = g/2$ and $v = f_3/6$), and ((3.104)) (with $u = g/2$ and $v = f_4/24$) to conclude that

$$\begin{aligned} &\left|\int_{-x_0}^{x_0} \cosh(f_1 x) e^{f_2 x^2/2}\left(e^{R_2(x)} - 1\right) dx\right| \\ &\quad = \left|\int_0^{x_0} \cosh(f_1 x) e^{f_2 x^2/2}\left(e^{R_2(x)} + e^{R_2(-x)} - 2\right) dx\right| \\ &\quad \leqslant \cosh(f_1 x_0)\int_0^{x_0} e^{-gx^2/2}\left|e^{R_2(x)} + e^{R_2(-x)} - 2\right| dx \\ &\quad \leqslant 2\cosh(f_1 x_0)\int_0^{x_0} e^{-gx^2/2}\left(\cosh\left(\frac{f_3|x|^3}{6}\right) - 1 + \sinh\left(\frac{f_4|x|^4}{24}\right)\right) dx \\ &\quad \leqslant 2\cosh(f_1 x_0)\operatorname{erf}\left(x_0\sqrt{\frac{g}{2}}\right)\left(\frac{8\sqrt{2} f_3^2 \beta_1(\mu_3)}{36 g^{7/2}} + \frac{4\sqrt{2} f_4 \beta_3(\mu_4)}{24 g^{5/2}}\right). \end{aligned}$$

For the third term, we utilise ((3.106)), ((3.103)) (with $u = g/2$ and $v = f_3/6$), and ((3.105)) (with $u = g/2$ and $v = f_4/24$) to conclude that

$$\begin{aligned}
&\left|\int_{-x_0}^{x_0} \sinh(f_1 x) e^{f_2 x^2/2} \left(e^{R_2(x)} - 1\right) dx\right| \\
&\qquad = \left|\int_{0}^{x_0} \sinh(f_1 x) e^{f_2 x^2/2} \left(e^{R_2(x)} - e^{R_2(-x)}\right) dx\right| \\
&\qquad \leqslant \int_{0}^{x_0} \sinh(f_1 x) e^{-gx^2/2} \left|e^{R_2(x)} - e^{R_2(-x)}\right| dx \\
&\qquad \leqslant 2 f_1 \cosh(f_1 x_0) \int_0^{x_0} x e^{-gx^2/2} \left(\sinh\left(\frac{f_3|x|^3}{6}\right) + \sinh\left(\frac{f_4|x|^4}{24}\right)\right) dx \\
&\qquad \leqslant 2 f_1 \cosh(f_1 x_0) \operatorname{erf}\left(x_0\sqrt{\frac{g}{2}}\right) \left(\frac{4\sqrt{2} f_3 \beta_2(\mu_3)}{6 g^{5/2}} + \frac{8 f_4 \beta_4(\mu_4)}{24 g^3}\right).
\end{aligned}$$

Combining the above bounds, we get

$$\begin{aligned}
&\left|\sqrt{\frac{g}{2\pi}} \int_{-x_0}^{x_0} \left(e^{f(x)} - e^{-gx^2/2}\right) dx\right| \leqslant \cosh(f_1 x_0) \operatorname{erf}\left(x_0\sqrt{\frac{g}{2}}\right) \\
&\qquad \times \left(\frac{|\operatorname{Im} f_2| + f_1^2}{2g} + \frac{4 f_3 \beta_1(\mu_3)}{9\sqrt{\pi} g^3} + \frac{f_4 \beta_3(\mu_4)}{3\sqrt{\pi} g^2} + \frac{4 f_1 f_3 \beta_2(\mu_3)}{3\sqrt{\pi} g^2} + \frac{\sqrt{2} f_1 f_4 \beta_4(\mu_4)}{3\sqrt{\pi} g^{5/2}}\right),
\end{aligned}$$

which is exactly the assertion of the lemma. □

As announced at the beginning of this section., our plan is to apply Lemma 3.8.1 to the function

$$x \mapsto \log \frac{e^{-imx} Q_n(re^{i(x+2\pi/3)})}{Q_n(re^{2\pi i/3})}$$

in order to get bounds on $\epsilon_{0,Q_n}(m, r)$. (The reader is reminded from Part B of the proof outline in Section 3.2 that $Q_n(q) = P_n^\delta(q)$ with $P_n(q)$ the "Borwein polynomial" from ((3.1)).) This application however requires upper and lower bounds for the various constants in Lemma 3.8.1, which we give next.

Lemma 3.8.2 *Suppose that $n \geqslant 400$, $m \in [3n, (\delta \deg P_n)/2]$, and r is the unique solution of the approximate saddle point equation ((3.19)) determined by n and m. Let*

$$f(\theta) := \delta\left(\log P_n(re^{i(\theta+2\pi/3)}) - \log P_n(re^{2\pi i/3}) - im\theta\right),$$

and let the constants f_j, $j = 1, 2, 3, 4$, be defined as in Lemma 3.8.1 with the bound θ_0 chosen as in ((3.25)). Then we have the following inequalities for the constants f_j:

$$f_1 < \frac{7}{40}\delta X_0(n, r), \tag{3.37}$$

$$\frac{1}{3}\delta X_2(n, r) \leqslant -\operatorname{Re} f_2 < \frac{3}{5}\delta X_2(n, r), \tag{3.38}$$

$$|\operatorname{Im} f_2| < \frac{1}{3}\delta X_1(n, r), \tag{3.39}$$

$$f_3 < \frac{2}{3}\delta X_3(n,r), \tag{3.40}$$

$$f_4 < \frac{18}{25}\delta X_4(n,r), \tag{3.41}$$

with the quantities $X_j(n,r)$ defined in ((3.18)).

Proof: Since all four constants are linear in f and therefore proportional to δ, we assume $\delta = 1$ in subsequent arguments without loss of generality.

We first give expressions respectively preliminary upper bounds on these constants. For f_1, we have

$$\begin{aligned} f_1 &= \left(\frac{d}{d\theta}\log P_n(re^{i(\theta+2\pi/3)})\right)\Big|_{\theta=0} - im \\ &= \operatorname{Re}\left(\frac{d}{d\theta}\log P_n(re^{i(\theta+2\pi/3)})\right)\Big|_{\theta=0} + i\operatorname{Re}\left(r\frac{d}{dr}\log P_n(re^{i(2\pi/3)})\right) - im \\ &= \frac{\sqrt{3}}{2}V_1(n,r), \end{aligned} \tag{3.42}$$

where we used ((3.13)) with $j = 1$ and the approximate saddle point equation ((3.19)) to get the last line. Still using ((3.13)), we have

$$f_2 = -\frac{1}{2}U_2(n,r) + \frac{\sqrt{3}i}{2}V_2(n,r), \tag{3.43}$$

$$f_3 \leqslant 3\int_0^1 (1-t)^2 \sup_{|\theta|\leqslant t\theta_0}\left(\frac{1}{2}\left|U_3(n,re^{i\theta})\right| + \frac{\sqrt{3}}{2}\left|V_3(n,re^{i\theta})\right|\right), \tag{3.44}$$

$$f_4 \leqslant 4\int_0^1 (1-t)^3 \sup_{|\theta|\leqslant t\theta_0}\left(\frac{1}{2}\left|U_4(n,re^{i\theta})\right| + \frac{\sqrt{3}}{2}\left|V_4(n,re^{i\theta})\right|\right). \tag{3.45}$$

Therefore the problem is reduced to proving upper and lower bounds for U_j and V_j.

UPPER AND LOWER BOUNDS FOR $U_2(n,r)$. The quantities U_j are comparable to the corresponding X_j; indeed, by comparing ((3.14)) and ((3.18)) and using ((3.88)), we immediately obtain

$$\frac{2}{3}X_2(n,r) \leqslant U_2(n,r) < \frac{6}{5}X_2(n,r),$$

which translates into

$$\frac{1}{3}X_2(n,r) \leqslant -\operatorname{Re} f_2 < \frac{3}{5}X_2(n,r),$$

establishing ((3.38)).

UPPER BOUNDS FOR $U_3(n,r)$ AND $U_4(n,r)$. Upper bounds for U_3 and U_4 can also be obtained by the same comparison. In fact, for arbitrary j we have

$$\begin{aligned} \sup_{|\theta|\leqslant t\theta_0}\left|U_j(n,re^{i\theta})\right| &\leqslant X_j(n,r)\sup_{|\theta|<t\theta_0}\sup_{0\leqslant k\leqslant 3n}\left|\frac{u_j(r^k e^{ik\theta})}{r^k e^{ik\theta}}\right| \\ &\leqslant X_j(n,r)\sup_{z\in S_{3tC_0}}\left|\frac{u_j(z)}{z}\right|, \end{aligned}$$

where S_ρ is defined in ((3.28)).

Remembering from ((3.25)) that $C_0 = 10/81$, we use Lemma 3.A.1(2) to conclude that

$$\begin{aligned}
3\int_0^1 (1-t)^2 \sup_{|\theta|\leqslant t\theta_0} |U_3(n, re^{i\theta})| &\leqslant 3X_3(n,r)\int_0^1 (1-t)^2 \sup_{z\in S_{3tC_0}} \left|\frac{u_3(z)}{z}\right| \\
&\leqslant \left(\frac{1}{8}\sup_{z\in S_{3C_0}}\left|\frac{u_3(z)}{z}\right| + \frac{7}{8}\sup_{z\in S_{3C_0/2}}\left|\frac{u_3(z)}{z}\right|\right) X_3(n,r) \\
&\leqslant \left(\frac{1}{8}\times 1.44 + \frac{7}{8}\times 1.3\right) X_3(n,r) = 1.3175 X_3(n,r),
\end{aligned}$$

and similarly

$$\begin{aligned}
4\int_0^1 (1-t)^3 \sup_{|\theta|\leqslant t\theta_0} |U_4(n, re^{i\theta})| &\leqslant 4X_4(n,r)\int_0^1 (1-t)^3 \sup_{z\in S_{3tC_0}} \left|\frac{u_4(z)}{z}\right| \\
&\leqslant \left(\frac{1}{16}\sup_{z\in S_{3C_0}}\left|\frac{u_4(z)}{z}\right| + \frac{15}{16}\sup_{z\in S_{3C_0/2}}\left|\frac{u_4(z)}{z}\right|\right) X_4(n,r) \\
&\leqslant \left(\frac{1}{16}\times 1.721 + \frac{15}{16}\times 1.409\right) X_4(n,r) = 1.4285 X_4(n,r).
\end{aligned}$$

A PRELIMINARY UPPER BOUND FOR $V_j(n,r)$. As opposed to the U_j's, the quantities V_j, as alternating sums, are expected to be much smaller than $X_j(n,r)$. Indeed, let $w_j(k,z) := k^j v_j(z^k)$. Using Lemma 3.A.5 for the function w_j, we see that

$$\begin{aligned}
|V_j(n,z)| &\leqslant \frac{1}{3}|w_j(3n,z) - w_j(0,z)| + \frac{2}{3}|w_j''(3n,z) - w_j''(0,z)| + \frac{11n}{96}\sup_{k\in[0,3n]}\left|w_j^{(4)}(k,z)\right| \\
&= \frac{1}{3}|w_j(3n,z)| + \frac{2}{3}|w_j''(3n,z)| + \frac{11n}{96}\sup_{k\in[0,3n]}\left|w_j^{(4)}(k,z)\right|, \qquad (3.46)
\end{aligned}$$

since direct calculations reveal that $w_j(0,z) = w_j''(0,z) = 0$ for $j = 1,2,3,4$.

In order to treat the derivatives of the functions w_j, we note that ((3.13)) implies that

$$\left(\frac{\partial}{\partial k}\right)^\ell v_j(z^k) = (\log z)^\ell v_{j+\ell}(z^k), \quad \text{for } \ell \geqslant 0. \qquad (3.47)$$

With this representation in mind, we proceed to give upper bounds for the right-hand side of ((3.46)) for $j = 1,2,3,4$, by making frequent use of inequalities from Lemma 3.A.1.

UPPER BOUND FOR $V_1(n,r)$. By using ((3.89)) and subsequently ((3.90)), we have

$$\frac{w_1(3n,r)/3}{X_0(n,r)} = \frac{1-r^3}{(-\log r)(1+r)}\frac{r^{3n-1}(-\log r^n)}{1-r^{9n}} \leqslant \frac{3}{2}\frac{r^{(3-1/400)n}(-\log r^n)}{1-r^{9n}} < 0.201$$

for the main term. Using ((3.47)) and ((3.93)), we get

$$|w_1''(3n,r)| = \frac{1}{3n}\left|2(\log r^{3n})v_2(r^{3n}) + (\log r^{3n})^2 v_3(r^{3n})\right| < \frac{1}{9n}$$

for the second derivative. On the other hand, using ((3.47)) and ((3.94)), we have

$$|w_1^{(4)}(k,r)| = |\log r|^3 \left|4v_4(r^k) + (\log r^k)v_5(r^k)\right| < \frac{9}{8}|\log r|^3$$

for the fourth derivative. Substitution of these bounds in ((3.46)) with $j = 1$, if combined with ((3.30)) and the fact from Lemma 3.5.1 that $|\log r| < |\log r_0| \leqslant \frac{2}{3}$, then yields

$$\begin{aligned}|V_1(n,r)| &\leqslant 0.201X_0(n,r) + \frac{2}{27n} + \frac{33n}{256}|\log r|^3 \\ &< \left(0.201 + \frac{2}{27\times 0.95n^{3/2}} + \frac{11}{288\times 0.95n}\right)X_0(n,r) < 0.202X_0(n,r).\end{aligned}$$

UPPER BOUND FOR $V_2(n,r)$. Similarly to above, using ((3.108)) in Lemma 3.A.7, and subsequently ((3.91)) and ((3.92)), we obtain

$$\begin{aligned}\frac{w_2(3n,r)/3}{X_1(n,r)} &\leqslant \frac{3(1-r^3)^2}{(1+2r+2r^3+r^4)(-\log r)^2}\frac{r^{3n-1}(1-r^{6n})(-\log r^n)^2}{(1-r^{9n})(1-r^{3n/2})(1+r^{3n}+r^{6n})} \\ &< \frac{9}{2}\frac{r^{(3-1/400)n}(1-r^{6n})(-\log r^n)^2}{(1-r^{9n})(1-r^{3n/2})(1+r^{3n}+r^{6n})} < 0.378\end{aligned}$$

for the main term. Using ((3.47)) and ((3.95)), we get

$$|w_2''(3n,r)| = \left|2v_2(r^{3n}) + 2(\log r^{3n})v_3(r^{3n}) + (\log r^{3n})^2 v_4(r^{3n})\right| < 0.21$$

for the second derivative. By ((3.47)) and ((3.96)), we infer

$$|w_2^{(4)}(k,r)| = |\log r|^2 \left|12v_4(r^k) + 8(\log r^k)v_5(r^k) + (\log r^k)^2 v_6(r^k)\right| < 3.61|\log r|^2$$

for the fourth derivative. Substitution of these bounds in ((3.46)) with $j = 2$, if combined with ((3.31)) and the earlier mentioned fact that $|\log r| < \frac{2}{3}$, then yields

$$\begin{aligned}V_2(n,r) &\leqslant 0.378X_1(n,r) + 0.14 + 0.42n|\log r|^2 \\ &< 0.378X_1(n,r) + 0.14 + 0.19 < 0.38X_1(n,r).\end{aligned}$$

UPPER BOUNDS FOR $V_3(n,re^{i\theta})$ AND $V_4(n,re^{i\theta})$. For these two quantities, instead of proving $V_j = O(X_{j-1})$ as above, we prove $V_j = o(X_j)$ as $n\to\infty$. Observe that Lemma 3.6.1(2) and ((3.47)) imply that for $a = 0,2,4$ we have

$$|w_j^{(a)}(k,re^{i\theta})| \leqslant r^k \sum_{\ell=0}^{a}\frac{a!}{\ell!}\binom{j}{a-\ell}k^{j-a+\ell}|\log re^{i\theta}|^\ell \sup_{z\in S_{3tC_0}}\left|\frac{v_{j+\ell}(z)}{z}\right|.$$

Therefore, by ((3.29)) and ((3.46)), we get

$$\begin{aligned}\sup_{|\theta|<t\theta_0}|V_j(n,re^{i\theta})| &\leqslant \frac{1}{3}(3n)^j r^{3n}\sup_{z\in S_{3tC_0}}\left|\frac{v_j(z)}{z}\right| \\ &\quad+\frac{2}{3}(3n)^j r^{3n}\sum_{\ell=0}^{2}\frac{2}{\ell!}\binom{j}{2-\ell}\frac{|\log re^{i\theta}|^\ell}{(3n)^{2-\ell}}\sup_{z\in S_{3tC_0}}\left|\frac{v_{j+\ell}(z)}{z}\right| \\ &+\frac{11n}{96}|\log re^{i\theta}|^{a-j}\sum_{\ell=0}^{4}\frac{24}{\ell!}\binom{j}{4-\ell}(j-a+\ell)^{j-a+\ell}(e^{-1}+3tC_0)^{j-a+\ell}\sup_{z\in S_{3tC_0}}\left|\frac{v_{j+\ell}(z)}{z}\right|.\end{aligned}$$

Here we put $t=1$ (thus raising the bound on the right-hand side since here $0\leqslant t\leqslant 1$). Substitution of the upper bounds from ((3.27)) (with $t=1$) and from Lemma 3.A.1(2) leads to

$$\begin{aligned}\sup_{|\theta|<\theta_0}|V_3(n,re^{i\theta})| &< (3n)^3r^{3n}\left(0.34+1.17n^{-1}+1.25n^{-3/2}+0.45n^{-2}\right)+45.1\sqrt{n} \\ &\leqslant 0.344(3n)^3r^{3n}+45.1\sqrt{n}, \\ \sup_{|\theta|<\theta_0}|V_4(n,re^{i\theta})| &< (3n)^4r^{3n}\left(0.34+3.04n^{-1}+3.40n^{-3/2}+0.91n^{-2}\right)+1135n \\ &\leqslant 0.349(3n)^3r^{3n}+1135n.\end{aligned}$$

We now note that for $j\in\mathbb{Z}^+$ we have

$$\frac{X_j(n,r)}{(3n)^jr^{3n}}\geqslant\frac{X_j(n,1)}{(3n)^j}>\frac{2}{j+1}(n-1).$$

Hence, by also using ((3.32)) and ((3.33)), we have

$$\begin{aligned}\frac{\sup_{|\theta|<\theta_0}|V_3(n,re^{i\theta})|}{X_3(n,r)} &< \frac{2\times 0.344}{n-1}+\frac{45.1}{16n^{3/2}}<\frac{5}{6n}, \\ \frac{\sup_{|\theta|<\theta_0}|V_4(n,re^{i\theta})|}{X_4(n,r)} &< \frac{5\times 0.349}{2(n-1)}+\frac{1135}{94n^{3/2}}<\frac{3}{2n}.\end{aligned}$$

By combining all the bounds above and using them in ((3.42))–((3.45)), we obtain

$$\begin{aligned}f_1 &< \frac{\sqrt{3}}{2}0.202X_0(n,r)<\frac{7}{40}X_0(n,r), \\ |\operatorname{Im}f_2| &< \frac{\sqrt{3}}{2}0.38X_1(n,r)<\frac{1}{3}X_1(n,r), \\ f_3 &< \left(\frac{1}{2}\times 1.3175+\frac{\sqrt{3}}{2}\times\frac{5}{6n}\right)X_3(n,r)<\frac{2}{3}X_3(n,r), \\ f_4 &< \left(\frac{1}{2}\times 1.4285+\frac{\sqrt{3}}{2}\times\frac{3}{2n}\right)X_4(n,r)<\frac{18}{25}X_4(n,r),\end{aligned}$$

thereby establishing the remaining inequalities. □

We are now ready for presenting, and proving, our upper bound for the peak error term $\epsilon_{0,P_n^\delta}(m,r)$ as defined in ((3.8)).

Lemma 3.8.3 *Let $n \geqslant 400$ and $\delta \in \{1,2,3\}$. Furthermore, for $m \in [3n, \delta(\deg P_n)/2]$, let $r = r_{n,m,\delta}$ be the solution of the approximate saddle point equation ((3.19)), and let θ_0 be the cutoff as defined in ((3.25)). Then we have the following upper bound for the peak error term $\epsilon_{0,P_n^\delta}(m,r)$:*

$$\epsilon_{0,P_n^\delta}(m,r) < (146.2\delta^{-1} + 6.46 + 0.124\delta)\frac{X_1(n,r)}{X_2(n,r)} + \frac{7.222}{\sqrt{\delta X_2(n,r)}}, \tag{3.48}$$

where the $X_j(n,r)$ are as defined in ((3.18)) and $g_{Q_n}(r)$ is defined in ((3.5)). Moreover, the right-hand side of ((3.48)) is decreasing with respect to r.

Proof: We apply Lemma 3.8.1 with $x_0 = \theta_0$ to the function

$$x \mapsto \log \frac{e^{-imx} Q_n(re^{i(x+2\pi/3)})}{Q_n(re^{2\pi i/3})}. \tag{3.49}$$

This produces a bound for $\epsilon_{0,P_n^\delta}(m,r)$ in terms of the quantities f_1, f_2, f_3, f_4, g and $\beta_1(\mu_3), \beta_2(\mu_3), \beta_3(\mu_4), \beta_4(\mu_4$ We now need to estimate the individual terms in ((3.35)) using the inequalities in Lemma 3.8.2 and Corollary 3.A.8, and the estimates for the particular values in Lemma 3.A.3. In order to justify the use of Lemma 3.A.3, we have to verify that $\mu_3 \leqslant 20/27$ and $\mu_4 \leqslant 2/3$. Indeed, using ((3.38)), ((3.40)), and the observation that, by definition, $g = -\operatorname{Re} f_2$ and $X_0(n,r) = r(1+r)(1-r^{3n})/(1-r^3)$, we have

$$\mu_3 = \frac{\theta_0 f_3}{3g} \leqslant \frac{2r(r+1)C_0 X_3(n,r)}{3X_0(n,r)X_2(n,r)} \leqslant 6C_0 = \frac{20}{27},$$

where we used ((3.114)). Similarly, using in addition ((3.41)), we get

$$\mu_4 = \sqrt{\frac{\theta_0^2 f_4}{8g}} \leqslant \sqrt{\frac{27C_0^2 X_4(n,r) r^2 (r+1)^2}{100 X_0^2(n,r) X_2(n,r)}} \leqslant \frac{27}{5} C_0 = \frac{2}{3},$$

where we used ((3.115)). Knowing these bounds, the application of Lemma 3.8.2 and Corollary 3.A.8 in order to bound the individual terms in ((3.35)) with our choices of function f and $x_0 = \theta_0$ is now straightforwardly done in the same way as the above estimations for μ_3 and μ_4.

The monotonicity with respect to r is proved by noticing that both X_2 and X_2/X_1 are increasing with respect to r; this is obvious for X_2, and we have

$$\frac{\partial}{\partial r}\frac{X_2(n,r)}{X_1(n,r)} = \frac{X_3(n,r)X_1(n,r) - X_2^2(n,r)}{rX_1^2(n,r)} \geqslant 0,$$

where the last inequality is a consequence of the Cauchy–Schwarz inequality. □

3.9 Bounding the tails

The goal of this section is to provide a bound for the tail error term $\epsilon_{1,Q_n}(r) = \epsilon_{1,P_n^\delta}(r)$. By the definition ((3.9)) of $\epsilon_{1,P_n^\delta}(r)$, what we need is upper bounds for $\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right|$. Phrased differently,

the objective is to get good lower bounds for the quantity

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| = -\sum_{\substack{k=1\\3\nmid k}}^{3n}\log\left|\frac{1-\left(re^{i\theta}\right)^k}{1-r^k e^{2\pi i/3}}\right|$$
$$= -\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3n}\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}} \tag{3.50}$$

in terms of θ, r, and n. Depending on the ranges of these parameters, we shall in fact establish two different lower bounds, presented in Lemmas 3.9.2 and 3.9.3 below. Lemma 3.9.1 provides a preliminary estimate that is used in the proof of Lemma 3.9.2. After these preparations, our bound for $\epsilon_{1,P_n^\delta}(r)$ is stated, and proved, in Lemma 3.9.4.

In the following, we shall use two possible lower bounds for the summand in ((3.50)):

1. For $x \in [-1/3, 1]$, we have $-\log(1-x) \geqslant x$. In this inequality, we replace x by $\frac{r^k}{1+r^k+r^{2k}}(1+2\cos(k\theta))$ to obtain

$$-\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}} \geqslant \frac{r^k}{1+r^k+r^{2k}}(1+2\cos(k\theta)). \tag{3.51}$$

2. For $z \in \mathbb{C}$ with $|z| \leqslant 1$, we have $|1-z^k| \leqslant k|1-z|$. Use of this inequality for $z = re^{i\theta}$ implies that

$$-\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}} \geqslant \log(1+r^k+r^{2k})-\log(1-2r\cos\theta+r^2)-2\log k. \tag{3.52}$$

Lemma 3.9.1 *For $r \in (0,1]$ and $\theta \in \mathbb{R}$, we have*

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant \frac{1}{3}\sum_{k=1}^{n} r^{3k}\,(1-\cos 3k\theta) - \frac{0.8}{|1-re^{i\theta}|}. \tag{3.53}$$

Proof: We use ((3.51)) to perform the following estimations:

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant \sum_{\substack{k=1\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}\left(\frac{1}{2}+\cos k\theta\right)$$
$$= \sum_{k=1}^{3n}\frac{r^k}{1+r^k+r^{2k}}\left(\frac{1}{2}+\cos k\theta\right) - \sum_{k=1}^{n}\frac{r^{3k}}{1+r^{3k}+r^{6k}}\left(\frac{1}{2}+\cos 3k\theta\right)$$
$$= \sum_{k=1}^{n}\frac{r^{3k}}{1+r^{3k}+r^{6k}}(1-\cos 3k\theta) + \sum_{k=1}^{3n}\frac{r^k\cos k\theta}{1+r^k+r^{2k}}$$
$$+\frac{1}{2}\sum_{k=1}^{n}\left(\frac{r^{3k-2}}{1+r^{3k-2}+r^{6k-4}} + \frac{r^{3k-1}}{1+r^{3k-1}+r^{6k-2}} - \frac{2r^{3k}}{1+r^{3k}+r^{6k}}\right)$$

$$\geqslant \frac{1}{3}\sum_{k=1}^{n} r^{3k}\,(1-\cos 3k\theta) + \sum_{k=1}^{3n} \frac{r^k \cos k\theta}{1+r^k+r^{2k}},$$

where we used $1/(1+r^{3k}+r^{6k}) \geqslant 1/3$ and the fact that the function $r^k/(1+r^k+r^{2k})$ is decreasing as a function in k. We apply Lemma 3.A.9 with $\varphi = 0$ to the last cosine sum to conclude that

$$\begin{aligned}
\left|\sum_{k=1}^{3n} \frac{r^k \cos k\theta}{1+r^k+r^{2k}}\right| &\leqslant \frac{1}{|1-re^{i\theta}|}\left((1-r)\sum_{k=1}^{3n}\frac{r^k}{1+r^k+r^{2k}} + 2\frac{r^{3n+1}}{1+r^{3n}+r^{6n}}\right)\\
&\leqslant \frac{1}{|1-re^{i\theta}|}\left((1-r)\int_0^{3n}\frac{r^k\,dk}{1+r^k+r^{2k}} + 2\frac{r^{3n}}{1+r^{3n}+r^{6n}}\right)\\
&= \frac{1}{|1-re^{i\theta}|}\left(\frac{1-r}{-\log r}\frac{2}{\sqrt{3}}\left(\frac{\pi}{3}-\arctan\frac{1+2r^{3n}}{\sqrt{3}}\right) + 2\frac{r^{3n}}{1+r^{3n}+r^{6n}}\right)\\
&< \frac{1}{|1-re^{i\theta}|}\left(\frac{2}{\sqrt{3}}\left(\frac{\pi}{3}-\arctan\frac{1+2r^{3n}}{\sqrt{3}}\right) + 2\frac{r^{3n}}{1+r^{3n}+r^{6n}}\right).
\end{aligned}$$

In order to complete the proof, we determine the maximum value of the function

$$f(s) := \frac{2\pi}{3\sqrt{3}} - \frac{2}{\sqrt{3}}\arctan\frac{1+2s}{\sqrt{3}} + \frac{2s}{1+s+s^2} \tag{3.54}$$

on $[0,1]$. Since $f'(s) = \frac{1-s-3s^2}{(1+s+s^2)^2}$ is decreasing with respect to s, we see that the unique maximum point of f is located at the unique zero of $f'(s)$ in $[0,1]$, namely $s_0 = (\sqrt{13}-1)/6$, giving a value of

$$f(s_0) \approx 0.7937 < 0.8. \qquad \square$$

In order to find a closed-form lower bound for the quantity $-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right|$, we apply Lemma 3.A.10 to the sum on the right-hand side of ((3.53)). In this manner, we obtain the following estimate.

Lemma 3.9.2 *If $\theta = 2h\pi/3 + \rho\frac{1-r^3}{1-r^{3n}}$ for some $h \in \mathbb{Z}$ and some $\rho \in \mathbb{R}$ such that $|\rho|\frac{1-r^3}{1-r^{3n}} \leqslant \pi/3$, then we have*

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant -\frac{0.8}{|1-re^{i\theta}|} + \frac{r^3(1+r^3)}{6}\frac{(1-r^{n/2})}{(1-r^3)}\left(1-\sqrt{\frac{1}{1+18\rho^2}}\right).$$

Remark: The slightly unusual looking scaling of the deviation of θ from $2h\pi/3$ above has its motivation in the desire of having the same scaling as in the definition of the cutoff θ_0; cf. ((3.25)) (remember that r depends on n and m!).

Proof (Proof of Lemma 3.9.2): Lemmas 3.9.1 and 3.A.10 (with the substitutions $r \mapsto r^3$, $\theta \mapsto 3\theta$) imply the inequality

$$\begin{aligned}
-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| &\geqslant \frac{1}{3}\sum_{k=1}^{n} r^{3k}\,(1-\cos 3k\theta) - \frac{0.8}{|1-re^{i\theta}|}\\
&\geqslant \frac{r^3}{3}\frac{1-r^{3n}}{1-r^3}\left(1-\sqrt{\frac{1}{1+4\kappa\tan^2(3\theta/2)}}\right) - \frac{0.8}{|1-re^{i\theta}|},
\end{aligned}$$

where

$$\kappa = \frac{(1+r^3)(1-r^{3n})(1-r^{n/2})}{(1-r^3)^2}.$$

We note that

$$\left|\tan\frac{3\theta}{2}\right| = \left|\tan\frac{3\rho}{2}\frac{1-r^3}{1-r^{3n}}\right| \geqslant \frac{3|\rho|}{2}\frac{1-r^3}{1-r^{3n}}$$

if $|\rho|\frac{1-r^3}{1-r^{3n}} \leqslant \pi/3$. We use this inequality to get rid of the tangent function:

$$1-\sqrt{\frac{1}{1+4\kappa\tan^2(3\theta/2)}} > 1-\sqrt{\frac{1}{1+\kappa\frac{9(1-r^3)^2}{(1-r^{3n})^2}\rho^2}}.$$

By making use of the inequality

$$1-\sqrt{\frac{1}{1+cx}} \geqslant c\left(1-\sqrt{\frac{1}{1+x}}\right)$$

for $0 < c \leqslant 1$ and $x > 0$, and by choosing

$$c = \frac{\kappa}{2}\frac{(1-r^3)^2}{(1-r^{3n})^2} = \frac{(1+r^3)}{2}\frac{(1-r^{n/2})}{(1-r^{3n})} \leqslant 1,$$

we arrive at the claimed result:

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant -\frac{0.8}{|1-re^{i\theta}|} + \frac{r^3(1+r^3)}{6}\frac{(1-r^{n/2})}{(1-r^3)}\left(1-\sqrt{\frac{1}{1+18\rho^2}}\right). \qquad \square$$

Note that the lower bound in Lemma 3.9.2 ceases to be effective when $|1-re^{i\theta}|$ is small. For this case, we present an alternative bound.

Lemma 3.9.3 *If $|1-re^{i\theta}| < \frac{1}{3}$, then we have*

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant \frac{1}{6}\frac{(r+r^2)(1-r^{3n})}{1-r^3} - 5.44.$$

Proof: Making reference to the sum representation ((3.50)), we define a cutoff

$$k_0 = \min\left\{\left\lfloor\frac{1}{3|1-re^{i\theta}|}\right\rfloor, n\right\}.$$

Note that the condition on $|1-re^{i\theta}|$ implies that $k_0 \geqslant 1$.

The part of the sum on the right-hand side of ((3.50)) where $k < 3k_0$ is treated by ((3.52)):

$$-\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3k_0}\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}}$$

$$\geqslant \frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3k_0}\Big(\log(1+r^k+r^{2k})-\log(1-2r\cos\theta+r^2)-2\log k\Big)$$

$$= -k_0\log(1-2r\cos\theta+r^2)-\log\frac{(3k)!}{3^k k!}+\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3k_0}\log(1+r^k+r^{2k}).$$

Now we use the inequality $\frac{(3k)!}{3^k k!} < \sqrt{3}(3k/e)^{2k}$, and the convexity of $k \mapsto \log(1+r^k+r^{2k})$, and obtain

$$\begin{aligned}
&-\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3k_0}\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}}\\
&> -k_0\log(1-2r\cos\theta+r^2)-\frac{1}{2}\log 3-2k_0(\log(3k_0)-1)+\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3k_0}\log(1+r^k+r^{2k})\\
&> -k_0\log(1-2r\cos\theta+r^2)-\frac{1}{2}\log 3-2k_0(\log(3k_0)-1)+k_0\log(1+r^{3k_0/2}+r^{3k_0})\\
&= -2k_0\log(3k_0|1-re^{i\theta}|)+2k_0-\frac{1}{2}\log 3+k_0\log(1+r^{3k_0/2}+r^{3k_0})\\
&\geqslant 2k_0-\frac{1}{2}\log 3+k_0\log(1+r^{3k_0/2}+r^{3k_0}),
\end{aligned}\tag{3.55}$$

where we used the definition of k_0 to get the last line.

For the part where $k > 3k_0$, we use ((3.51)), split the sum according to the residue classes of k modulo 3, and apply Lemma 3.A.9 to each subsum, to get

$$\begin{aligned}
-\frac{1}{2}\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}\log\frac{1-2r^k\cos(k\theta)+r^{2k}}{1+r^k+r^{2k}} &\geqslant \frac{1}{2}\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}\frac{r^k(1+2\cos(k\theta))}{1+r^k+r^{2k}}\\
&\geqslant \left(\frac{1}{2}-\frac{1-r^3}{|1-r^3e^{3i\theta}|}\right)\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}-\frac{4}{|1-r^3e^{3i\theta}|}\frac{r^{3n}}{1+r^{3n}+r^{6n}}.
\end{aligned}\tag{3.56}$$

We first observe that in the case where $k_0 = n$ the estimate ((3.55)) provides the lower bound

$$2n-\frac{1}{2}\log 3 \geqslant \frac{(r+r^2)(1-r^{3n})}{1-r^3}-\frac{1}{2}\log 3 > \frac{1}{6}\frac{(r+r^2)(1-r^{3n})}{1-r^3}-5.44,$$

as desired.

Therefore, we assume $0 < k_0 < n$ from now on. By combining ((3.55)) and ((3.56)), we obtain

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant \left(\frac{1}{2}-\frac{1-r^3}{|1-r^3e^{3i\theta}|}\right)\sum_{\substack{k=3k_0\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}$$
$$+(2+\log(1+r^{3k_0/2}+r^{3k_0}))k_0-\frac{4}{|1-r^3e^{3i\theta}|}\frac{r^{3n}}{1+r^{3n}+r^{6n}}-\frac{1}{2}\log 3. \quad (3.57)$$

We split the right-hand side of ((3.57)) into several parts:

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| \geqslant I_1+I_2+I_3+I_4,$$

where

$$I_1=\frac{1}{2}\sum_{\substack{k=3k_0\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}+\frac{1}{3}k_0,$$
$$I_2=-\frac{1-r^3}{|1-r^3e^{3i\theta}|}\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}},$$
$$I_3=k_0(\log(1+r^{3k_0/2}+r^{3k_0})-\log(1+r^{3n/2}+r^{3n})),$$
$$I_4=\left(\frac{5}{3}+\log(1+r^{3n/2}+r^{3n})\right)k_0-\frac{4}{|1-r^3e^{3i\theta}|}\frac{r^{3n}}{1+r^{3n}+r^{6n}}-\log\sqrt{3}.$$

For I_1 we have

$$I_1\geqslant\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}\geqslant\frac{1}{2}\sum_{\substack{k=1\\3\nmid k}}^{3n}\frac{r^k}{3}=\frac{1}{6}\frac{(r+r^2)(1-r^{3n})}{1-r^3}.$$

It should be noted that the right-hand side in this inequality is exactly the main term in the desired lower bound. Consequently, what we need to prove is $I_2+I_3+I_4\geqslant -5.44$.

From here on, we write $z=re^{i\theta}$ for simplicity of notation.

We first deal with I_4. By utilising the inequality

$$\left|\log(1+\sqrt{s}+s)-\frac{3s}{1+s+s^2}\right|\leqslant\frac{1}{10},\qquad 0\leqslant s\leqslant 1,$$

for $s=r^{3n}$, we infer that

$$I_4\geqslant\left(\frac{47}{30}+\frac{3r^{3n}}{1+r^{3n}+r^{6n}}\right)k_0-\frac{12(k_0+1)}{|1+z+z^2|}\frac{r^{3n}}{1+r^{3n}+r^{6n}}-\log\sqrt{3}.$$

Now we note that for $0<k_0<n$ we have

$$k_0=\left\lfloor\frac{1}{3|1-z|}\right\rfloor\geqslant\frac{1}{3|1-z|}-1.$$

We use this in the above estimate for I_4 to get

$$\begin{aligned}
I_4 &\geqslant \frac{47}{30}\left(\frac{1}{3|1-z|}-1\right)+\frac{3r^{3n}\left(\frac{1}{3|1-z|}-1\right)}{1+r^{3n}+r^{6n}} \\
&\qquad\qquad -\frac{12}{3|1-z|\cdot|1+z+z^2|}\frac{r^{3n}}{1+r^{3n}+r^{6n}}-\log\sqrt{3} \\
&> \left(\frac{47}{30}-\left(\frac{12}{|1+z+z^2|}-3\right)\frac{r^{3n}}{1+r^{3n}+r^{6n}}\right)\frac{1}{3|1-z|}-\log\sqrt{3}-\frac{47}{30}-\frac{3r^{3n}}{1+r^{3n}+r^{6n}} \\
&\geqslant \left(\frac{47}{30}-\left(\frac{12}{|1+z+z^2|}-3\right)\frac{1}{3}\right)\frac{1}{3|1-z|}-\log\sqrt{3}-\frac{77}{30} \\
&= \left(\frac{77}{30}-\frac{4}{|1+z+z^2|}\right)\frac{1}{3|1-z|}-\log\sqrt{3}-\frac{77}{30}.
\end{aligned}$$

In order to bound I_2, we argue that

$$\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}\frac{r^k}{1+r^k+r^{2k}}\leqslant\sum_{\substack{k=3k_0+1\\3\nmid k}}^{3n}r^k=\frac{(r+r^2)(r^{3k_0}-r^{3n})}{1-r^3}\leqslant\frac{2(r^{3k_0}-r^{3n})}{1-r^3},$$

and consequently

$$I_2\geqslant-\frac{2}{|1-z^3|}(r^{3k_0}-r^{3n}).$$

Writing $h(x)=\frac{6}{|1+z+z^2|}x-\log(1+\sqrt{x}+x)$, we combine the above estimate for I_2 into one for I_2+I_3:

$$\begin{aligned}
I_2+I_3 &\geqslant -\frac{2}{|1-z^3|}(r^{3k_0}-r^{3n}) \\
&\qquad\qquad +\left(\frac{1}{3|1-z|}-1\right)\left(\log(1+r^{3k_0/2}+r^{3k_0})-\log(1+r^{3n/2}+r^{3n})\right) \\
&= -\Big(h(r^{3k_0})-h(r^{3n})\Big)\frac{1}{3|1-z|}-\left(\log(1+r^{3k_0/2}+r^{3k_0})-\log(1+r^{3n/2}+r^{3n})\right) \\
&\geqslant -\Big(h(r^{3k_0})-h(r^{3n})\Big)\frac{1}{3|1-z|}-\log 3 \\
&\geqslant -\left(\max_{0\leqslant x\leqslant 1}h(x)-\min_{0\leqslant x\leqslant 1}h(x)\right)\frac{1}{3|1-z|}-\log 3.
\end{aligned}$$

Note that the function h is convex with respect to x. Hence, the maximum of $h(x)$ is either $h(0)$ or $h(1)$. Since $|1+z+z^2|\leqslant 3$, we have $h(1)\geqslant 2-\log 3>0=h(0)$. Therefore,

$$\max_{0\leqslant x\leqslant 1}h(x)=h(1)=\frac{6}{|1+z+z^2|}-\log 3.$$

On the other hand, again using that $|1+z+z^2| \leqslant 3$, we have

$$\min_{0\leqslant x\leqslant 1} h(x) \geqslant \min_{0\leqslant x\leqslant 1}(2x - \log(1+\sqrt{x}+x)) \approx -0.1496 > -\frac{3}{20},$$

which in turn implies

$$I_2 + I_3 \geqslant -\left(\frac{6}{|1+z+z^2|} - \log 3 + \frac{3}{20}\right)\frac{1}{3|1-z|} - \log 3.$$

Combining all the inequalities above, we obtain

$$I_2 + I_3 + I_4 \geqslant \left(\frac{29}{12} + \log 3 - \frac{10}{|1+z+z^2|}\right)\frac{1}{3|1-z|} - \frac{3}{2}\log 3 - \frac{77}{30}.$$

We write $u = |1-z|$. By the assumptions of the lemma, we have $u \in [0, 1/3]$. We claim that $|1+z+z^2| \geqslant 3 - 3u + u^2$ for $u \in [0, 1/3]$. This can be proved by writing $1 - z = ue^{i\varphi}$ for some φ, expressing z in terms of u and φ, and minimising $|1+z+z^2|$ with respect to φ. In addition, we point out that the function $u \mapsto \left(\frac{29}{12} + \log 3 - \frac{10}{3-3u+u^2}\right)\frac{1}{3u}$ is decreasing with respect to u, and therefore

$$\begin{aligned} I_2 + I_3 + I_4 &\geqslant \left(\frac{29}{12} + \log 3 - \frac{10}{3-3u+u^2}\right)\frac{1}{3u} - \frac{3}{2}\log 3 - \frac{77}{30} \\ &\geqslant \frac{29}{12} + \log 3 - \frac{90}{19} - \frac{3}{2}\log 3 - \frac{77}{30} \\ &= -\frac{1857}{380} - \frac{1}{2}\log 3 > -5.44, \end{aligned}$$

as desired. □

We are now ready to provide, and prove, an explicit upper bound for the tail error term $\epsilon_{1,P}(n,r)$ as defined in ((3.9)).

Lemma 3.9.4 *Suppose that $n \in \mathbb{Z}^+$, and that r_0 is defined as in ((3.20)). Then, for $\delta \in \{1,2,3\}$ and $r \in (r_0, 1]$, we have*

$$\begin{aligned} \epsilon_{1,P_n^\delta}(r) < \frac{\sqrt{54\delta}}{\sqrt{5\pi}} \Bigg/ \operatorname{erf}\sqrt{\frac{40\delta(1-r^{3n})}{243(1-r^3)}} \\ \times \left(4\left(\frac{1-r^{3n}}{1-r^3}\right)^{1/2}\int_{10/81}^{4} \exp\left(\frac{0.8\delta}{\sqrt{3}-(1+3\rho)(-\log r_0)} - \delta\phi(n,r,\rho)\right) d\rho \right. \\ \left. + 2\pi\left(\frac{1-r^{3n}}{1-r^3}\right)^{3/2} \exp(5.44\delta - \delta\phi(n,r,4))\right), \quad (3.58) \end{aligned}$$

where

$$\phi(n,r,\rho) := \frac{r^3(1+r^3)}{6}\left(1 - \sqrt{\frac{1}{1+18\rho^2}}\right)\frac{(1-r^{n/2})}{(1-r^3)}.$$

Moreover, for $n > 546$, the right-hand side of ((3.58)) is decreasing with respect to r.

Proof: Lemmas 3.9.2 and 3.9.3 imply that

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| > -\frac{0.8}{|1-re^{i\theta}|} + \phi(n,r,|\rho|),$$
$$\text{for } \theta = \pm\frac{2\pi i}{3} + \rho\frac{1-r^3}{1-r^{3n}} \text{ and } |1-re^{i\theta}| \geqslant \frac{1}{3}, \tag{3.59}$$

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right| > -5.44 + \phi(n,r,+\infty), \qquad \text{for } |1-re^{i\theta}| < \frac{1}{3}. \tag{3.60}$$

For $\theta := \pm\frac{2\pi i}{3} + \rho\frac{1-r^3}{1-r^{3n}}$, we have

$$\begin{aligned}
|1-re^{i\theta}| &= \left|(1-e^{\pm 2\pi i/3}) + (e^{\pm 2\pi i/3} - e^{i\theta}) + (e^{i\theta} - re^{i\theta})\right| \\
&\geqslant |1-e^{\pm 2\pi i/3}| - |e^{\pm 2\pi i/3} - e^{i\theta}| - |e^{i\theta} - re^{i\theta}| \\
&\geqslant \sqrt{3} - |\rho|\frac{1-r^3}{1-r^{3n}} - (1-r) \geqslant \sqrt{3} - |\rho|\frac{1-r_0^3}{1-r_0^{3n}} - (1-r_0) \\
&\geqslant \sqrt{3} - (3|\rho|+1)(-\log r_0),
\end{aligned} \tag{3.61}$$

where we used that $r \in (r_0, 1]$ to get the next-to-last line, and ((3.26)) to obtain the last line.

Here, in order to estimate the integral in ((3.9)), we divide the tail part I_{tail} into two disjoint subsets. Namely, we define

$$I_{\text{tail1}} := \left\{\pm 2\pi/3 + \rho\frac{1-r^3}{1-r^{3n}} : C_0 < |\rho| < 4\right\}$$

and the complementary subset $I_{\text{tail2}} := I_{\text{tail}} \backslash I_{\text{tail1}}$. The set I_{tail1} consists of four distinct intervals. By ((3.59)) and ((3.61)), the integral over these intervals can be estimated by

$$\begin{aligned}
&\int_{I_{\text{tail1}}} \left|\frac{Q_n(re^{i\theta})}{Q_n(re^{2\pi i/3})}\right| d\theta \\
&\qquad < 4\frac{1-r^3}{1-r^{3n}} \int_{C_0}^{4} \exp\left(\frac{0.8\delta}{\sqrt{3}-(1+3|\rho|)(-\log r_0)} - \delta\phi(n,r,\rho)\right) d\rho.
\end{aligned} \tag{3.62}$$

For the remaining part of I_{tail}, $I_{\text{tail2}} := I_{\text{tail}} \backslash I_{\text{tail1}}$, we note that the quantity

$$-\log\left|\frac{P_n(re^{i\theta})}{P_n(re^{2\pi i/3})}\right|$$

can be bounded below by either $-2.4 + \phi(n,r,4)$ (if $|1-re^{i\theta}| \geqslant \frac{1}{3}$, using ((3.59))) or $-5.44 + \phi(n,r,+\infty)$ (if $|1-re^{i\theta}| < \frac{1}{3}$, using ((3.60))), and a common lower bound for the two cases can be chosen as $-5.44 + \phi(n,r,4)$. This implies that

$$\int_{I_{\text{tail2}}} \left|\frac{Q_n(re^{i\theta})}{Q_n(re^{2\pi i/3})}\right| d\theta < 2\pi \exp(5.44\delta - \delta\phi(n,r,4)). \tag{3.63}$$

By combining the two bounds ((3.62)) and ((3.63)), we obtain the following upper bound for the integral in ((3.9)):

$$\int_{I_{\text{tail}}} \left| \frac{Q_n(re^{i\theta})}{Q_n(re^{2\pi i/3})} \right| d\theta < 4\frac{1-r^3}{1-r^{3n}} \int_{10/81}^{4} \exp\left(\frac{0.8\delta}{\sqrt{3}-(1+3|\rho|)(-\log r_0)} - \delta\phi(n,r,\rho) \right) d\rho + 2\pi \exp(5.44\delta - \delta\phi(n,r,4)).$$

We recall that the definition ((3.9)) of $\epsilon_{1,Q_n}(r)$ contains the factor

$$\sqrt{g_{Q_n}(r)} \Big/ \operatorname{erf}\left(\theta_0\sqrt{g_{Q_n}(r)/2}\right)$$

in addition to the left-hand side of the above inequality. We note that, using the upper bound for $-\operatorname{Re} f_2$ in ((3.38)) and the inequality ((3.113)), we have

$$g_{P_n^\delta}(r) < \frac{108\delta}{5}\left(\frac{1-r^{3n}}{1-r^3}\right)^3.$$

Therefore, using the fact that $x/\operatorname{erf} x$ is increasing with respect to x and recalling the definition of θ_0 in ((3.25)), we obtain

$$\epsilon_{1,P_n^\delta}(r) < \frac{\sqrt{54\delta}}{\sqrt{5\pi}} \Bigg/ \operatorname{erf}\left(\sqrt{\frac{40\delta(1-r^{3n})}{243(1-r^3)}}\right) \times \left(4\left(\frac{1-r^{3n}}{1-r^3}\right)^{1/2} \int_{10/81}^{4} \exp\left(\frac{0.8\delta}{\sqrt{3}-(1+3\rho)(-\log r_0)} - \delta\phi(n,r,\rho)\right) d\rho + 2\pi\left(\frac{1-r^{3n}}{1-r^3}\right)^{3/2} \exp(5.44\delta - \delta\phi(n,r,4))\right),$$

as desired.

It remains to show that the right-hand side of ((3.58)) is decreasing with respect to r. To this end, we first note that the factor $1/\operatorname{erf}\left(\sqrt{\frac{40\delta(1-r^{3n})}{243(1-r^3)}}\right)$ is decreasing with respect to r.

We claim that the other factor on the right-hand side of ((3.58)) is also decreasing with respect to r. To see this, let $r_1, r_2 \in [r_0, 1]$ such that $r_1 < r_2$. We then use Lemma 3.A.12 with r replaced by r^3 and

$$\lambda = C\delta\frac{r_1^3(1+r_1^3)}{6}\left(1-\sqrt{\frac{1}{1+18\rho^2}}\right), \tag{3.64}$$

to get

$$\frac{1-r_2^{3n}}{1-r_2^3}\exp\left(-C\delta\frac{r_1^3(1+r_1^3)}{r_2^3(1+r_2^3)}\phi(n,r_2,\rho)\right) \leqslant \frac{1-r_1^{3n}}{1-r_1^3}\exp\left(-C\delta\phi(n,r_1,\rho)\right),$$

provided

$$546 \geqslant 6 + \frac{36}{\lambda}. \tag{3.65}$$

(Recall that $n > 546$ by assumption.)

Let us for the moment assume that the condition ((3.65)) is satisfied. Then, since $r_2^3(1+r_2^3) > r_1^3(1+r_1^3)$, we obtain

$$\frac{1-r_2^{3n}}{1-r_2^3}\exp\left(-C\delta\phi(n,r_2,\rho)\right) \leqslant \frac{1-r_1^{3n}}{1-r_1^3}\exp\left(-C\delta\phi(n,r_1,\rho)\right), \tag{3.66}$$

again provided ((3.65)) holds. It can be checked that, for $C = 2$, the inequality ((3.65)) holds for $\frac{10}{81} \leqslant \rho \leqslant 4$. Therefore, setting $C = 2$ in ((3.66)) and taking square roots of both sides, we obtain

$$\left(\frac{1-r_2^{3n}}{1-r_2^3}\right)^{1/2}\exp\left(-\delta\phi(n,r_2,\rho)\right) \leqslant \left(\frac{1-r_1^{3n}}{1-r_1^3}\right)^{1/2}\exp\left(-\delta\phi(n,r_1,\rho)\right), \quad \text{for } \frac{10}{81} \leqslant \rho \leqslant 4. \tag{3.67}$$

For $C = 2/3$, the inequality ((3.65)) only holds for $\rho = 4$. By doing these substitutions in ((3.66)) and raising both sides to the power $3/2$, we arrive at

$$\left(\frac{1-r_2^{3n}}{1-r_2^3}\right)^{3/2}\exp\left(-\delta\phi(n,r_2,4)\right) \leqslant \left(\frac{1-r_1^{3n}}{1-r_1^3}\right)^{3/2}\exp\left(-\delta\phi(n,r_1,4)\right). \tag{3.68}$$

The inequalities ((3.67)) and ((3.68)) together show that the second factor on the right-hand side of ((3.58)) is indeed also decreasing in r.

It remains to justify the use of Lemma 3.A.12, that is, of the validity of the condition ((3.65)).

- We note that $n > 546$ implies that

  $$r_0^3 = \exp\left(-3\sqrt{\frac{4\delta}{27n}}\right) > \exp\left(-3\sqrt{\frac{12}{27\times 546}}\right) > \frac{11}{12},$$

  and consequently

  $$\frac{r_1^3(1+r_1^3)}{6} \geqslant \frac{r_0^3(1+r_0^3)}{6} > 0.292.$$

- Therefore, with the choice $C = 2$ and $10/81 \leqslant \rho \leqslant 4$, the constant λ in ((3.64)) is at least

  $$2 \times 0.292\delta(1-(1+18(10/81)^2)^{-1/2}) > \delta/15.$$

  Hence, the condition ((3.65)) holds, which confirms ((3.67)). On the other hand, with the choice $C = 2/3$ and $\rho = 4$, the constant λ in ((3.64)) is at least

  $$2/3 \times 0.292\delta(1-(1+18\times 4^2)^{-1/2}) > \delta/6.$$

  Hence, again, the condition ((3.65)) is satisfied, confirming ((3.68)).

- The condition in Lemma 3.A.12 on the range of r is verified by noting that

$$-\log r^3 < \frac{\sqrt{\delta}}{9\sqrt{5}} < \frac{\sqrt{\delta}}{20} \leqslant \frac{\delta}{20} < \frac{8}{9}\lambda.$$

□

3.10 Completion of the proofs

In this section, we combine the results of the two previous sections to prove the First and Second Borwein Conjecture and "two thirds" of the cubic Borwein conjecture. We begin by giving a result that allows us to control the argument of $P_n(re^{2\pi i/3})$. As mentioned in Part D of Section 3.2, this is needed for accomplishing Task (2) below ((3.11)).

Lemma 3.10.1 *For $n \in \mathbb{Z}^+$, $\arg P_n(re^{2\pi i/3})$ is increasing with respect to r. Moreover, for $r \in (0,1]$ and $n \in \mathbb{Z}^+$, we have $\arg P_n(re^{2\pi i/3}) \in (-\pi/18, 0]$.*

Proof: For $x \in \mathbb{R}$, define

$$f(r,x) := \arg(1 - r^x e^{2\pi i/3}) = -\arctan \frac{\sqrt{3}r^x}{r^x + 2}.$$

By elementary manipulations, we have

$$\begin{aligned}
\arg P_n(re^{2\pi i/3}) &\equiv \sum_{k=1}^{n} \left(\arg(1 - r^{3k-2}e^{2\pi i/3}) + \arg(1 - r^{3k-1}e^{-2\pi i/3})\right) \pmod{2\pi} \\
&= \sum_{k=1}^{n} \left(\arg(1 - r^{3k-2}e^{2\pi i/3}) - \arg(1 - r^{3k-1}e^{2\pi i/3})\right) \\
&= -\sum_{k=1}^{n} \left(f(r,3k-1) - f(r,3k-2)\right).
\end{aligned}$$

We claim that $f(r,3k-1) - f(r,3k-2)$ is decreasing with respect to r, and that

$$\sum_{k=1}^{n} \left(f(r,3k-1) - f(r,3k-2)\right) \in [0, \pi/18).$$

In order to see this, we note that

$$\sum_{k=1}^{n} \left(f(r,3k-1) - f(r,3k-2)\right) = \sum_{k=1}^{n} \int_{3k-2}^{3k-1} f_x(r,x)\,dx,$$

where as usual $f_x(r,x) = \frac{\partial}{\partial x} f(r,x)$. Both the lower bound of 0 and the monotonicity with respect to r follow from the expression

$$f_x(r,x) = \frac{\sqrt{3}r^x(-\log r)}{2(1 + r^x + r^{2x})}.$$

In order to prove the upper bound of $\pi/18$, we define $g(r,x) := \sum_{k\in\mathbb{Z}} f_x(r, 3k+x)$ and claim that

$$\int_1^2 g(r,x)\,dx \leqslant \frac{1}{3}\int_0^3 g(r,x)\,dx. \tag{3.69}$$

If we assume the truth of this inequality for a moment, then, since f_x is even with respect to x, we see that

$$\begin{aligned}\sum_{k=1}^{n}\left(f(r,3k-1)-f(r,3k-2)\right) &< \frac{1}{2}\sum_{k\in\mathbb{Z}}\left(f(r,3k-1)-f(r,3k-2)\right)\\ &= \frac{1}{2}\int_1^2 g(r,x)\,dx \leqslant \frac{1}{6}\int_0^3 g(r,x)\,dx = \frac{1}{6}\int_{-\infty}^{\infty} f_x(r,x)\,dx\\ &= \frac{1}{6}f(r,x)\Big|_{-\infty}^{+\infty} = \pi/18,\end{aligned}$$

as required.

Hence, it remains to verify ((3.69)). As a matter of fact, this inequality can be proved by a Fourier expansion of $g(r,x)$. To be precise, we define

$$g_k(r) := \int_0^3 g(r,x)\cos(2\pi kx/3)\,dx = \int_{\mathbb{R}} f_x(r,x)\cos(2\pi kx/3)\,dx,$$

so that

$$g(r,x) = \frac{1}{3}g_0(r) + \frac{2}{3}\sum_{k=1}^{\infty} g_k(r)\cos(2k\pi x/3).$$

To get an explicit expression for $g_k(r)$, we note that, since $f_x(r,x)$ is even, we may express the Fourier coefficients as

$$g_k(r) = \int_{\mathbb{R}} f_x(r,x)\exp(2\pi kix/3)\,dx.$$

We integrate the function $f_x(r,x)\exp(2\pi kix/3)$ (clockwise) along a rectangular contour with corners located at $\pm M$ and $\pm M - 2\pi i/(-\log r)$. In the limit as $M\to\infty$, the integral along the two vertical parts of the contour converges to zero, while the two parts of the integral along the horizontal parts of the contour are proportional to each other. More precisely, we may conclude that the integral along this rectangular contour, in the limit as $M\to\infty$, is equal to

$$\left(\exp\left(4k\pi^2/(-3\log r)\right)-1\right)\cdot g_k(r).$$

The integrand has exactly two poles inside this rectangle, namely at $x = -2\pi i/(-3\log r)$ and at $x = -4\pi i/(-3\log r)$, with residues equal to $i\exp(4k\pi^2/(-9\log r))$ and to $-i\exp(8k\pi^2/(-9\log r))$, respectively. Therefore we obtain that

$$g_k(r) = \frac{\pi}{1+2\cosh\left(\frac{4k\pi^2}{9(-\log r)}\right)}.$$

We are now in the position to accomplish a proof of ((3.69)) by employing the above facts:

$$\begin{aligned}\left(\frac{1}{3}\int_0^3 - \int_1^2\right) g(r,x)\,dx &= \frac{2}{3}\sum_{k=1}^{\infty} g_k(r)\left(\frac{1}{3}\int_0^3 - \int_1^2\right)\cos(2k\pi x/3)\,dx \\ &= \sum_{k=1}^{\infty}\frac{8(-1)^{k-1}g_k(r)\sin^3(k\pi/3)}{3k\pi} \\ &= \frac{\sqrt{3}}{\pi}\left(g_1(r) - \frac{g_2(r)}{2} + \frac{g_4(r)}{4} - \frac{g_5(r)}{5} + \cdots\right) > 0,\end{aligned}$$

where the last inequality is due to the fact that $g_k(r)$ is decreasing with respect to k. □

With concrete bounds on $\arg P_n(re^{2\pi i/3})$ proven, all three pieces of the Borwein puzzle are now in place, and we can now present the announced proofs of the First and Second Borwein Conjecture, and of "two thirds" of the Cubic Borwein Conjecture.

We begin with the (in view of [Wan22]: alternative) proof of the First Borwein Conjecture. In the arguments below, we always use r_m to denote the solution of the approximate saddle point equation ((3.22)) (that depends on n, m, and δ).

Theorem 3.10.2 *The First Borwein Conjecture, Conjecture 3.1.1, is true.*

Proof: We prove this claim by verifying ((3.11)) for "large" n, with the help of the various bounds and inequalities we have derived, and by a direct computation for "small" n, using the computer.

By Lemma 3.10.1, we have $\arg P_n(r_m e^{2\pi i/3}) \in [-\pi/18, 0]$. Hence, by Lemma 3.A.13, we infer

$$\left|2\cos\left(\arg P_n(r_m e^{2\pi i/3}) - 2m\pi/3\right)\right| \geqslant 2\min\{1/2, \cos(7\pi/18)\} > 0.684. \tag{3.70}$$

Furthermore, for $n \geqslant 5300$ and $m \in [3n, \deg P_n]$ (so that $r_m \in (r_0, 1]$ by Lemma 3.5.1), we use Lemma 3.8.3 and Lemma 3.9.4 to see that

$$\epsilon_{0,P_n}(m, r_m) < 0.407, \qquad \epsilon_{1,P_n}(r_m) < 0.275. \tag{3.71}$$

Comparing the bounds in ((3.70)) and ((3.71)), we see that ((3.11)) holds. Hence, by ((3.10)), the First Borwein Conjecture is true for $n \geqslant 5300$.

A full computer verification for $n \leqslant 7000$ of the First Borwein Conjecture has already been done, cf. [Wan22, Sec. 13]. (But see also Remark 4 below.) This finishes the proof. □

Next we finish the proof of the Second Borwein Conjecture.

Theorem 3.10.3 *The Second Borwein Conjecture, Conjecture 3.1.2, is true.*

Proof: Again, we prove this claim by verifying ((3.11)) for "large" n and a direct computation for "small" n.

By Lemma 3.10.1, we have $\arg P_n^2(r_m e^{2\pi i/3}) \in [-\pi/9, 0]$. Then, by Lemma 3.A.13, we may conclude that

$$\left|2\cos\left(\arg P_n^2(r_m e^{2\pi i/3}) - 2m\pi/3\right)\right| \geqslant \left|2\cos\left(\pi/3 - \arg P_n^2(r_m e^{2\pi i/3})\right)\right|. \tag{3.72}$$

In particular, we have

$$\left|2\cos\left(\arg P_n^2(r_m e^{2\pi i/3}) - 2m\pi/3\right)\right| \geqslant 2\cos(4\pi/9) > 0.347. \tag{3.73}$$

Furthermore, for $n \geqslant 7000$ and $m \in [3n, (\deg P_n^2)/2]$ (so that $r_m \in (r_0, 1]$ by Lemma 3.5.1), we use Lemma 3.8.3 and Lemma 3.9.4 to see that

$$\epsilon_{0,P_n^2}(m, r_m) < 0.262, \qquad \epsilon_{1,P_n^2}(r_m) < 0.079. \tag{3.74}$$

Comparing the bounds in ((3.73)) and ((3.74)), we see that ((3.11)) holds. Hence, by ((3.10)), the Second Borwein Conjecture is true for $n \geqslant 7000$.

We now discuss the range $546 < n < 7000$. Again referring to Lemma 3.10.1, the argument $\arg P_n(r_m e^{2\pi i/3})$ is increasing as a function in r_m. Consequently, the right-hand side of ((3.72)) is also increasing in r_m. On the other hand, we note that, according to Lemma 3.8.3 and Lemma 3.9.4, for $n > 546$ the left-hand side of ((3.11)) with $\delta = 2$ has an upper bound that is decreasing with respect to r_m. Therefore, for $n > 546$, there exists $r^* = r^*(n)$ such that ((3.11)) with $\delta = 2$ holds for $r \in [r^*, 1]$. For each specific n, $r^*(n)$ can be calculated by any method for the numerical approximation of zeroes of a function with sufficient accuracy. If we substitute $r^*(n)$ in ((3.22)) then we can compute a corresponding $m^*(n)$. Now ((3.10)) implies that, for $m \in [m^*(n), (\deg P_n^2)/2]$, the coefficient $[q^m]P_n^2(q)$ has the predicted sign.

It turns out that $m^*(n) < 25281$ in the region $546 < n < 7000$. Hence, it remains to calculate the first 25281 coefficients of $P_n^2(q)$ for $546 < n < 7000$, and *all* coefficients of $P_n^2(q)$ for $n \leqslant 546$. We programmed the corresponding calculations using C with the GMP library [Gt02]. They took less than one day on a personal laptop computer. □

Remark: A line of argument similar to the one in the preceding proof makes it possible to reduce the amount of calculation reported in the proof of Theorem 3.10.2 significantly. Namely, this line of argument shows that only a full calculation of the coefficients of $P_n(q)$ for $1 \leqslant n \leqslant 546$, and a calculation of the coefficients $[q^m]P_n(q)$ for $m \in [0, 34168]$ and $546 < n < 5300$ is needed. The corresponding calculations took about 4 hours on a personal laptop computer, as opposed to the computations reported in [Wan22, Sec. 13] which took 2 days using a multiple-core cluster.

Finally, the theorem below says that "two thirds" of the Cubic Borwein Conjecture, Conjecture 3.1.3, are true.

Theorem 3.10.4 *The coefficient* $[q^m]P_n^3(q)$ *is positive if* $3|m$, *and is negative if* $m \leqslant 3(\deg P_n)/2$ *and* $m \equiv 1 \pmod 3$.

Remark: While it may seem at first sight that the statement in Theorem 3.10.4 is just "one half" of Conjecture 3.1.3, it is indeed "two thirds" of that conjecture. To understand this, we should recall that $P_n(q)$ is palindromic, and therefore also $P_n^3(q)$. Consequently, Theorem 3.10.4 also implies that the coefficient $[q^m]P_n^3(q)$ is negative if $m \geqslant 3(\deg P_n)/2$ and $m \equiv 2 \pmod 3$.

Proof (Proof of Theorem 3.10.4): The proof and calculations are completely analogous to the ones of Theorems 3.10.2 and 3.10.3, with the key difference being that the constraint $m \equiv 0, 1 \pmod 3$ implies that, again using Lemma 3.A.13, a lower bound for $\left|2\cos\left(\arg P_n^\delta(r_m e^{2\pi i/3}) - 2m\pi/3\right)\right|$ is actually 1. We calculate for $n \geqslant 3150$ that

$$\epsilon_{0,P_n^3}(m, r_m) < 0.335, \qquad \epsilon_{1,P_n^3}(r_m) < 0.614,$$

and perform a full calculation of the coefficients of $P_n^3(q)$ for $1 \leqslant n \leqslant 546$, as well as a calculation of the coefficients $[q^m]P_n^3(q)$ for $m \in [0, 8864]$ for $546 < n < 3150$. Since we have $\sup_{546<n<3150} m^*(n) < 8864$, this suffices for the proof. □

Remark: The reason why we cannot prove Conjecture 3.1.3 for $m \equiv 2 \pmod 3$ with $m \leqslant 3(\deg P_n)/2$ is that the right-hand side of ((3.11)) can get arbitrarily close to 0 since, by Lemma 3.10.1, we can only conclude that $\arg P_n^3(r_m e^{2\pi i/3}) \in [-\pi/6, 0]$. We will elaborate on this in Item (1) of the next, and final, section.

3.11 Discussion and outlook

In this paper, we proved the First and Second Borwein Conjecture, and — partially — a Cubic Borwein Conjecture, by developing an asymptotic framework that allowed us to verify these conjectures for "large" n, meaning that in each case a specific n_0 of very modest size was given, and it was proved that the corresponding conjecture held for $n \geqslant n_0$. Together with a direct calculation for the remaining "small" n using a computer, the proofs could be completed. We are convinced that this framework can be further enhanced and extended to a machinery that is capable of establishing the positivity/negativity of coefficients in more general products/quotients of q-shifted factorials. We discuss this perspective in this section.

We start our discussion by going back to the Cubic Borwein Conjecture, Conjecture 3.1.3, and work out what prevented us at this stage to come up with a full proof (see Item (1)). Indeed, that "failure" strongly points out one direction where our method needs refinement. Subsequently, we turn our attention to the Third Borwein Conjecture and other "Borwein-like" sign pattern conjectures that one finds in the literature, in particular a conjecture of Ismail, Kim and Stanton (see Item (2)). As we argue there, we have no doubt that our ideas that we presented here will lead to substantial progress, if not full proof, of these. Then we report on computer experiments that we performed that led us to discover new Borwein-type conjectures for the moduli 4 and 7 and make other intriguing observations concerning sign patterns in such polynomials (see Item (3)). Bressoud's conjecture that was mentioned in the introduction is a vast generalisation of the First Borwein Conjecture. Although, from the outset, it does not seem that our method has anything to say about that conjecture, we show that Bressoud's alternating sum expression can be converted into a double contour integral of a product of q-shifted factorials. Therefore our ideas do apply. Whether progress can be made in this way remains to be seen. We close this section by a discussion of the "nature" of the Borwein Conjectures, whether they should be considered as "combinatorial" or as "analytic".

(1) Which are the obstacles to complete the proof of the Cubic Borwein Conjecture, Conjecture 3.1.3? It may have come somewhat unexpected that, with the machinery developed here, we proved "only" "two thirds" of Conjecture 3.1.3 and left non-positivity of the coefficients of q^{3m+2} in $P_n^3(q)$, $0 \leqslant m < (\deg P_n)/2$, (and consequently also the non-positivity of the coefficients of q^{3m+1} in $P_n^3(q)$, $(\deg P_n)/2 \leqslant m \leqslant \deg P_n$), open.

The main reason for this "failure", as mentioned in Remark 6, is that the right-hand side of ((3.11)) can get arbitrarily close to 0. Indeed, by applying Lemma 3.A.5 to the function $x \mapsto f(r, x)$ defined in the proof of Lemma 3.10.1, we are able to obtain a much more accurate estimate for

the argument of $P_n(re^{2\pi i/3})$, namely

$$\arg P_n(re^{2\pi i/3}) = -\frac{\pi}{18} + \frac{1}{3}\arctan\frac{\sqrt{3}r^{3n}}{2+r^{3n}} + O(n^{-1}r^{3n}). \tag{3.75}$$

This implies that, for $\delta = 3$ and $m \equiv 2 \pmod 3$, the right-hand side of ((3.11)) is equal to

$$\begin{aligned} 2\cos\left(3\arg P_n(re^{2\pi i/3}) + 2\pi/3\right) &= 2\cos\left(\frac{\pi}{2} + \arctan\frac{\sqrt{3}r^{3n}}{2+r^{3n}}\right) + O(n^{-1}r^{3n}) \\ &= \frac{\sqrt{3}\,r^{3n}}{\sqrt{1+r^{3n}+r^{6n}}} + O(n^{-1}r^{3n}), \end{aligned}$$

which, for values of $r = \exp(-\Theta(n^{-1/2}))$ near the cutoff r_0, is of the order $\exp(-\Theta(n^{1/2}))$. In comparison, the bound for the peak error term $\epsilon_{0,P_n^\delta}(m, r_m)$ that results from Lemma 3.8.3 is of the order $O(n^{-1/2})$ for $r = \exp(-\Theta(n^{-1/2}))$. Therefore, in this regime for r, the inequality ((3.11)) does not hold in the $n \to \infty$ limit. Roughly speaking, this issue is caused by the addition of the two peak contributions in ((3.4)), which are complex conjugates of each other (cf. Part C in Section 3.2), but in this case happen to have real part very close to zero (approaching zero as $n \to \infty$), and therefore largely cancel each other. What this observation implies is that the peak contribution — and thus the coefficient of $P_n^3(q)$ itself — is "unusually" small in this case. This is also mirrored by the earlier observed fact (cf. the end of Section 3.3) that the coefficient $[q^m]P_\infty^3(q)$ is always zero if $m \equiv 2 \pmod 3$. So, again roughly speaking, what is at stake here is to determine the "next" term(s) in the asymptotic expansion of the peak part of the integral in order to allow for a more precise estimate of the error made by approximating the peak part by a Gaußian integral.

(2) WHAT ABOUT OTHER "BORWEIN-LIKE" CONJECTURES? As we said in the introduction, *three* Borwein Conjectures were reported in [And95]: Conjectures 3.1.1 and 3.1.2, and the *Third Borwein Conjecture*, an analogue of the First Borwein Conjecture (Conjecture 3.1.1) in which the modulus 3 is replaced by 5.

Conjecture 3.11.1 (P. BORWEIN) For all positive integers n, the sign pattern of the coefficients in the expansion of the polynomial $S_n(q)$ defined by

$$S_n(q) := \frac{(q;q)_{5n}}{(q^5;q^5)_n}$$

is $+----+----+----\cdots$, with the same convention concerning zero coefficients as in Conjectures 3.1.1 and 3.1.2.

It should be clear that the approach that we presented in this paper can also be applied to this conjecture, in adapted form. In order to show that the "first few" and the "last few" coefficients of $S_n(q)$ obey the predicted sign pattern (necessary for completing the analogue of Part A in Section 3.2), we would quote [And95, Eq. (2.5)] with $p = 5$,

$$\frac{(q;q)_\infty}{(q^5;q^5)_\infty} = \sum_{k=-2}^{2}(-1)^k q^{k(3k+1)/2}\frac{(q^{75};q^{75})_\infty\,(q^{40+15k};q^{75})_\infty\,(q^{35-15k};q^{75})_\infty}{(q^5;q^5)_\infty}, \tag{3.76}$$

which Andrews derived by using Euler's pentagonal number theorem and Jacobi's triple product

identity. For the contour integral representation of $[q^m]S_n(q)$ (the analogue of Part B in Section 3.2), we would again choose a circle of radius r, $0 < r \leqslant 1$. Here, we would have to deal with *four* approximate saddle points (analogue of Part C in Section 3.2): $re^{\pm 2\pi i/5}$ and $re^{\pm 4\pi i/5}$, with r being a solution of the obvious approximate saddle point equation analogous to ((3.19)). All these four approximate dominant saddle points would contribute peaks of the same asymptotic order to the contour integral. Clearly, the estimations in Sections 3.8 and 3.9 would have to be adapted accordingly. We expect however that this approach can prove that the coefficients $[q^{5m}]S_n(q)$, $[q^{5m+1}]S_n(q)$, $[q^{5m+2}]S_n(q)$ have the predicted signs for $n \leqslant m \leqslant \frac{1}{10}\deg(S_n(q))$. On the other hand, in the case of the coefficients $[q^{5m+3}]S_n(q)$ and $[q^{5m+4}]S_n(q)$ we would face the same difficulty as we do for the coefficients $[q^{3m+2}]P_n^3(q)$ as discussed above: from ((3.76)) we see that the coefficients $[q^{5m+3}]S_\infty(q)$ and $[q^{5m+4}]S_\infty(q)$ are all zero, and this indicates that the corresponding coefficients in $S_n(q)$ are relatively small, and therefore it will require much more accurate estimations in order to show that these coefficients are negative.

Ismail, Kim and Stanton [IKS99, Conj. 1 in Sec. 7] generalised the First Borwein Conjecture, Conjecture 3.1.1, in a direction different from the earlier mentioned Bressoud Conjecture.

Conjecture 3.11.2 (Ismail, Kim and Stanton) Let a and K be relatively prime positive integers, $1 \leqslant a \leqslant K/2$, with K being odd. Put

$$\prod_{i=0}^{n-1}(1-q^{a+iK})(1-q^{K-a+iK}) = \sum_{m\geqslant 0} b_m q^m.$$

The sign of b_m is determined by m modulo K. More precisely, if $m \equiv \pm(2l+1)a \ (mod\ K)$ for some l with $0 \leqslant l < K/2$, then $b_m \leqslant 0$, otherwise $b_m \geqslant 0$.

Our approach is certainly tailored for an attack on this conjecture. As already pointed out in [IKS99], the "infinite" case (the analogue of Part A) follows easily from the Jacobi triple product identity. For the contour integral representation of the coefficients we would again choose a circle, with approximate saddle points of the modulus of the integrand at $re^{\pm 2\pi i b/K}$, where $2ab \equiv 1 \bmod K$. The fact that this conjecture contains additional parameters — namely K and a — may be an obstacle for a full proof, in particular in the checking part (for small n) of our approach. A proof of Conjecture 3.11.2 for sufficiently large n should however definitely be feasible.

It is reasonable to believe that, with the approach in this paper, the sign-pattern problem for a general polynomial of the form

$$Q_n(q) := \prod_j (q^{\alpha_j};q^K)_n\,(q^{K-\alpha_j};q^K)_n \tag{3.77}$$

can be reduced to an "infinite case" analogous to what is proved in Section 3.3, and an inequality analogous to ((3.11)), where the error terms tend to zero uniformly as $n \to \infty$. Naturally, the sign pattern of the polynomial coefficients would be determined by analogues of the right-hand side of ((3.11)), which would turn out to be essentially a sum of the cosines of "arguments" over all dominant peaks. Analogous to ((3.75)), the arguments of these peak values can be well approximated as functions of the quantity r^{Kn}. Here, the r is the solution of an approximate saddle point equation, which at the same time connects it to an index m, and thus to the coefficient of q^m in the polynomial ((3.77)). Below we list a rough correspondence of the orders

of magnitude of the quantities r and m, which can in principle be obtained by arguments similar to those in Section 3.5:

Coefficients	r	r^{Kn}	m
near the cutoff	$\exp(-\Theta(n^{-1/2}))$	$\exp(-\Theta(n^{1/2}))$	$O(n)$
somewhere in the "interior"	$\exp(-\Theta(n^{-1}))$	$\Theta(1)$	$\Theta(n^2)$
the central coefficient	1	1	$\frac{1}{2}(\deg Q_n) = \Theta(n^2)$

From the table above we can see that, as the index m ranges from $\Theta(n)$ — where the coefficients of $Q_n(q)$ start to differ from $Q_\infty(q)$ — to $\Theta(n^2)$ — where we find the central coefficient of $Q_n(q)$ —, the quantity r^{Kn} is expected to take any values from 0 to 1. This allows us to predict the sign patterns for polynomials or power series of the form ((3.77)) by the following process:

Step 1. Identify the pair(s) of dominant peaks among $\varphi(K)/2$ candidates located near primitive K-th roots of unity, where $\varphi(\,.\,)$ denotes Euler's totient function.

Step 2. For each pair of dominant peaks (say, located at arguments $\pm\theta$ where $0 < \theta < \pi$), calculate the arguments of the function values at these places and approximate them by functions of r^{Kn}. Using Maclaurin summation techniques similar to Lemma 3.A.5, we claim that each factor $(q^{\alpha_j}, q^{K-\alpha_j}; q^K)_n$ in ((3.77)) contributes an amount of

$$-\frac{K-2\alpha_j}{K}\arctan\frac{(1-r^{Kn})\cot(\alpha_j\theta/2)}{1+r^{Kn}} + O(r^{Kn}n^{-1}) \tag{3.78}$$

to the argument of $Q_n(re^{i\theta})$.

Step 3. Therefore, the analogue of the right-hand side of ((3.11)) would (approximately) be

$$\sum_\ell 2\cos\left(-im\theta_\ell - \sum_j \frac{K-2\alpha_j}{K}\arctan\frac{(1-r^{Kn})\cot(\alpha_j\theta_\ell/2)}{1+r^{Kn}}\right), \tag{3.79}$$

where the outer sum is over all pairs of arguments $\pm\theta_\ell$ of dominant peaks, and the inner sum is over all factors in ((3.77)). By substituting different values for r^{Kn} (remember that r depends on m) and different residue classes of m modulo K, we can read off the general behaviour of $[q^m]Q_n(q)$ from ((3.79)).

(3) More conjectures. We have performed extensive computer calculations in order to see whether, apart from the new Cubic Borwein Conjecture, Conjecture 3.1.3, there are more sign pattern phenomena in Borwein-type polynomials that have not been discovered yet. Our most striking findings are the following two conjectures. In the first of the two, we use the truth notation $\chi(\mathcal{A}) = 1$ if $\mathcal{A}$ is true and $\chi(\mathcal{A}) = 0$ otherwise.

Conjecture 3.11.3 (A modulus 4 "Borwein Conjecture") Let n be a positive integer and $\delta \in \{1, 2, 3\}$. Furthermore, consider the expansion of the polynomial

$$\frac{(q;q)_{4n}^\delta}{(q^4;q^4)_n^\delta} = \sum_{m=0}^{D} c_m^{(\delta)}(n)q^m,$$

which has degree $D = 6\delta n^2$. Then

$$c_{4m}^{(\delta)}(n) \geqslant 0 \quad \text{and} \quad c_{4m+2}^{(\delta)}(n) \leqslant 0, \quad \text{for all } m \text{ and } n, \tag{3.80}$$

while

$$c_{4m+1}^{(\delta)}(n) \leqslant 0, \quad \text{for} \begin{cases} 0 \leqslant m \leqslant \frac{1}{8}(6\delta n^2 - 8), & \text{if } n \text{ is even,} \\ 0 \leqslant m \leqslant \frac{1}{8}(6\delta n^2 - 8 + 2\delta), & \text{if } n \text{ is odd,} \end{cases} \tag{3.81}$$

and

$$c_{4m+3}^{(\delta)}(n) \geqslant 0, \quad \text{for} \begin{cases} 0 \leqslant m \leqslant \frac{1}{8}(6\delta n^2 - 8), & \text{if } n \text{ is even,} \\ 0 \leqslant m \leqslant \frac{1}{8}(6\delta n^2 - 6\delta + 8\chi(\delta = 3)), & \text{if } n \text{ is odd,} \end{cases} \tag{3.82}$$

with the exception of two coefficients: for $\delta = 1$ and $n = 5$, we have $c_{71}^{(1)}(5) = -1$ and $c_{79}^{(1)}(5) = 1$.

Remark: Roughly speaking, what the above conjecture says is that all coefficients $c_{4m}^{(\delta)}(n)$ are non-negative, all coefficients $c_{4m+2}^{(\delta)}(n)$ are non-positive, the "first half" of the coefficients $c_{4m+1}^{(\delta)}(n)$ is non-positive, and the "first half" of the coefficients $c_{4m+3}^{(\delta)}(n)$ is non-negative (with the mentioned exceptions in the case where $n = 5$). Since the polynomial $(q;q)_{4n}/(q^4;q^4)_n$ is palindromic for even n and skew-palindromic for odd n, we have

$$c_m^{(\delta)}(n) = (-1)^{\delta n} c_{6\delta n^2 - m}^{(\delta)}(n).$$

Consequently, the statements ((3.81)) and ((3.82)) imply that the coefficients $c_{4m+1}^{(\delta)}(n)$ are non-negative for m outside the ranges given in ((3.81)) (with two exceptions for $n = 5$), and similarly the coefficients $c_{4m+3}^{(\delta)}(n)$ are non-positive for m outside the ranges given in ((3.82)).

Conjecture 3.11.4 (A MODULUS **7** "BORWEIN CONJECTURE") For positive integers n, consider the expansion of the polynomial

$$\frac{(q;q)_{7n}}{(q^7;q^7)_n} = \sum_{m=0}^{21n^2} d_m(n) q^m.$$

Then

$$d_{7m}(n) \geqslant 0 \quad \text{and} \quad d_{7m+1}(n), d_{7m+3}(n), d_{7m+4}(n), d_{7m+6}(n) \leqslant 0, \quad \text{for all } m \text{ and } n, \tag{3.83}$$

while

$$d_{7m+5}(n) \begin{cases} \geqslant 0, & \text{for } m \leqslant 3\alpha(n)n^2, \\ \leqslant 0, & \text{for } m > 3\alpha(n)n^2, \end{cases} \tag{3.84}$$

where $\alpha(n)$ seems to stabilise around 0.302.

Remark: (1) Since the polynomial $(q;q)_{7n}/(q^7;q^7)_n$ is palindromic, the above conjecture makes also a prediction for the signs of the coefficients $d_{7m+2}(n)$.

(2) The existence and approximate position of the sign change for the coefficients of q^m with $m \equiv 2, 5 \pmod 7$ predicted in ((3.84)) can in fact be explained by the general procedure for approaching proofs of sign patterns in the polynomial ((3.77)), here specialised to $K = 7$ and

$\alpha_j = j$ for $j = 1, 2, 3$. As a matter of fact, the function $(q;q)_{7n}/(q^7;q^7)_n$ has three pairs of dominant peaks (of the same order of magnitude) located at $re^{\pm 2\pi i\ell/7}$ for $\ell = 1, 2, 3$. We set $\alpha_j = j$, for $j = 1, 2, 3$, and $\theta_\ell = 2\pi i\ell/7$, for $\ell = 1, 2, 3$, in ((3.79)) to conclude that, for $m \equiv 5 \pmod 7$, the sum ((3.79)) evaluates to $2\sqrt{7}\cos(3\pi/7)$ for $r^{7n} = 0$, and to -1 for $r^{7n} = 1$. This indicates a sign change somewhere in the middle. More precisely, in this case we can pinpoint the zero of ((3.79)) as $r^{7n} \approx 0.6089$. For convenience, let us write $s_0 := 0.6089$. The analogue of the approximate saddle point equation ((3.19)) for our situation here can be calculated as

$$\frac{1}{3}\sum_{\substack{k=1\\ 7\nmid k}}^{7n} k\frac{r^k - 7r^{7k} + 6r^{8k}}{(1-r^k)(1-r^{7k})} = 2m.$$

Therefore, for $r^{7n} = s_0$, making the substitution $k \mapsto 7nu$, we get

$$\begin{aligned}\lim_{n\to\infty}\frac{m}{21n^2} &= \lim_{n\to\infty}\frac{7}{18(7n)^2}\left(\sum_{k=1}^{7n} k\frac{r^k - 7r^{7k} + 6r^{8k}}{(1-r^k)(1-r^{7k})} - \sum_{k=1}^{n} 7k\frac{r^{7k} - 7r^{49k} + 6r^{56k}}{(1-r^{7k})(1-r^{49k})}\right)\\ &= \frac{7}{18}\times\frac{6}{7}\int_0^1 u\frac{s_0^u - 7s_0^{7u} + 6s_0^{8u}}{(1-s_0^u)(1-s_0^{7u})}du \approx 0.30214,\end{aligned}$$

which explains the occurrence of the constant 0.302 in Conjecture 3.11.4.

Many similar conjectures could be proposed. For example, it seems that the coefficient of q^{6m} in $(q;q)_{6n}/(q^6;q^6)_n$ is non-negative for all m, the coefficient of q^{6m+3} in $(q;q)_{6n}/(q^6;q^6)_n$ is non-positive for all m, while, for large enough n, the other sequences of coefficients in congruence classes modulo 6 of the exponents of q seem to satisfy sign patterns similar to the one in ((3.84)). Similarly, for $\delta \in \{2, 3\}$, it seems that the coefficient of q^{5m} in $(q;q)_{5n}^\delta/(q^5;q^5)_n^\delta$ is non-negative for all m, while, for large enough n, the other sequences of coefficients in congruence classes modulo 5 of the exponents of q seem to also satisfy sign patterns similar to the one in ((3.84)).

(4) THE BRESSOUD CONJECTURE. Inspired by sum representations of the decomposition polynomials $A_n(q), B_n(q), C_n(q)$ defined in ((3.2)) which Andrews found by the use of the q-binomial theorem (cf. [And95, Eqs. (3.4)–(3.6)]), Bressoud [Bre96, Conj. 6] came up with the following far-reaching generalisation of the First Borwein Conjecture. For the statement of Bressoud's conjecture we need to introduce the usual q-binomial coefficients, defined by

$$\begin{bmatrix} A \\ B \end{bmatrix}_q := \begin{cases} \dfrac{(q;q)_A}{(q;q)_B\,(q;q)_{A-B}}, & \text{for } 0 \leqslant B \leqslant A,\\ 0, & \text{otherwise.}\end{cases}$$

Conjecture 3.11.5 (BRESSOUD) Suppose that $M, N \in \mathbb{Z}^+$, α and β are positive rational numbers, and K is a positive integer such that αK and βK are integers. If $1 \leqslant \alpha + \beta \leqslant 2K + 1$ *(*with strict inequalities if $K = 2$*)* and $\beta - K \leqslant n - M \leqslant K - \alpha$, then the polynomial

$$\sum_{j=-\infty}^{\infty} (-1)^j q^{j(K(\alpha+\beta)j + K(\alpha-\beta))/2} \begin{bmatrix} M+N \\ M+Kj \end{bmatrix}_q \tag{3.85}$$

has non-negative coefficients.

Conjecture 3.1.1 turns out to be a special case of this conjecture for the choices $\alpha = 5/3$, $\beta = 4/3$ and $K = 3$.

To this day, Bressoud's conjecture has only been proved when $\alpha, \beta \in \mathbb{Z}$ (corresponding to a result of Andrews et al. [And+87] on partitions with restricted hook differences), and some sporadic parametric infinite families (see [Ber20b; BW05; War01; War03]).

If one tries a direct attack on proving non-negativity of the coefficients of the polynomial ((3.85)) using contour integral methods (in the style of [Wan22], where however different sum representations of $A_n(q), B_n(q), C_n(q)$ were used as starting point), then one would discover that a large amount of cancellation is going on in ((3.85)) which is impossible to control.

Instead, we could apply the q-binomial theorem [**GaRaAA**] to express the q-binomial coefficient as

$$\begin{bmatrix} A \\ B \end{bmatrix}_q = q^{-\binom{B}{2}} [z^B](-z;q)_A.$$

This leads to

$$\begin{aligned}
&\sum_{j=-\infty}^{\infty} (-1)^j q^{j(K(\alpha+\beta)j+K(\alpha-\beta))/2} \begin{bmatrix} M+N \\ M+Kj \end{bmatrix}_q \\
&\quad = \sum_{j=-\infty}^{\infty} [z^{M+Kj}](-1)^j q^{\frac{1}{2}j(K(\alpha+\beta)j+K(\alpha-\beta))-\binom{M+Kj}{2}} (-z;q)_{M+N} \\
&\quad = [z^M] q^{-\binom{M}{2}} (-z;q)_{M+N} \sum_{j=-\infty}^{\infty} (-1)^j q^{\frac{1}{2}(j^2K(\alpha+\beta-K)+jK(\alpha-\beta+1-M))} z^{-Kj}. \qquad (3.86)
\end{aligned}$$

If we assume that $|q| < 1$ and $\alpha + \beta > K$, then we may now apply the Jacobi triple product identity (cf. [**GaRaAA**]),

$$\sum_{j=-\infty}^{\infty} (-1)^j q^{\binom{j}{2}} u^j = (q, u, q/u; q)_\infty, \qquad (3.87)$$

where $(\alpha_1, \alpha_2, \ldots, \alpha_s; q)_\infty$ is short for the product $\prod_{i=1}^{s} (\alpha_i; q)_\infty$. As a consequence, we obtain

$$\begin{aligned}
\sum_{j=-\infty}^{\infty} (-1)^j q^{j(K(\alpha+\beta)j+K(\alpha-\beta))/2} \begin{bmatrix} M+N \\ M+Kj \end{bmatrix}_q &= [z^M] q^{-\binom{M}{2}} (-z;q)_{M+N} \\
&\quad \cdot (q^{K(\alpha+\beta-K)}, z^{-K} q^{K(2\alpha-K+1-M)/2}, z^K q^{K(2\beta-K-1+M)/2}; q^{K(\alpha+\beta-K)})_\infty.
\end{aligned}$$

The coefficient of q^m of the right-hand side can be represented as a double contour integral over z and q of a product of (finite and infinite) shifted q-factorials and is therefore — at least in principle — amenable to the ideas that we developed in this paper.

If $\alpha + \beta < K$, then we would assume $|q| > 1$ and try an analogous approach. On the other hand, if $\alpha + \beta = K$, then the sum in ((3.86)) can be evaluated by summing a geometric series.[8] Hence, again, we obtain an expression that can be converted into a double contour integral that is amenable to the ideas developed in this paper.

[8] The reader should keep in mind that, for fixed M and N, the sum over j is a finite sum.

(5) ARE THE BORWEIN CONJECTURES COMBINATORIAL OR ANALYTIC IN NATURE? This question is somewhat on the provocative side. It seems that it has been commonly believed that the Borwein Conjecture(s) is (are) combinatorial in nature, in the sense that the most promising approaches for a proof are combinatorial, may it be by an injective argument, or by q-series manipulations, or by a combination of the two. However, we believe that by now considerable evidence has accumulated for the feeling that this might have been a misconception. On the superficial level, one must simply admit that, despite considerable effort, until now "combinatorial" attacks have not led to any progress on the Borwein Conjectures (but undeniably to further intriguing discoveries). By contrast, the first proof of the First Borwein Conjecture in [Wan22] has been accomplished using analytic methods, as well as the proof in this paper. More substantially, several of the more recently discovered related or similar results and conjectures, such as Conjecture 3.11.4 (cf. in particular Remark 8(2)), the many conjectures by Bhatnagar and Schlosser in [BS19], or Kane's result [Kan04] that we used in Section 3.3 seem to indicate that *"typically"* such sign pattern results hold for "large" n, and in *some* cases — such as in the case of the Borwein Conjectures — they *"accidentally"* also hold for "small" n. This is not to say that we do not think that it is desirable to find a combinatorial proof of, say, the First Borwein Conjecture. On the contrary! However, one should be aware that such a proof would most likely not have anything to say about the Second Borwein Conjecture or the Cubic Borwein Conjecture, while, by our analytic approach, we could do the First and Second Borwein Conjecture (and large parts of the Cubic Borwein Conjecture) — so-to-speak — in one stroke. Obviously, the last word in this matter has not yet been spoken.

3.A Appendix: auxiliary inequalities

Here we collect several auxiliary inequalities of very technical nature that we need in the main text. We put them here so as to not disturb the flow of arguments in the main text.

3.A.1 Bounds for certain rational functions in s and $\log s$

In the lemma below, we collect various bounds for the auxiliary functions $u_j(z)$ and $v_j(z)$ from Section 3.4. They are used ubiquitously in Sections 3.5, 3.8, and 3.9.

Lemma 3.A.1 *Suppose that $u_j(z)$ and $v_j(z)$, $j \in \mathbb{Z}^+$, are as defined in* ((3.16)) *and* ((3.17)). *Furthermore, for $\rho \in \mathbb{R}^+$, let the region S_ρ be defined as in* ((3.28)).

(1) *For $s \in (0,1]$, we have the following inequalities:*

$$\frac{u_1(s)}{s} \leqslant \frac{2}{\sqrt{3}}, \quad \frac{2}{3} \leqslant \frac{u_2(s)}{s} < \frac{6}{5}, \tag{3.88}$$

$$\frac{1-s^3}{(-\log s)(1+s)} \leqslant \frac{3}{2}, \tag{3.89}$$

$$\frac{s^{3-1/400}(-\log s)}{1-s^9} < 0.134, \tag{3.90}$$

$$\frac{(1-s^3)^2}{(-\log s)^2(1+2s+2s^3+s^4)} \leqslant \frac{3}{2}, \tag{3.91}$$

$$\frac{s^{3-1/400}(1-s^6)(-\log s)^2}{(1-s^9)(1-s^{3/2})(1+s^3+s^6)} < 0.084, \tag{3.92}$$

$$\left|2(\log s)v_2(s) + (\log s)^2 v_3(s)\right| < \frac{1}{3}, \tag{3.93}$$

$$\left|4v_4(s) + (\log s)v_5(s)\right| < \frac{9}{8}, \tag{3.94}$$

$$\left|2v_2(s) + 2(\log s)v_3(s) + (\log s)^2 v_4(s)\right| < 0.21, \tag{3.95}$$

$$\left|12v_4(s) + 8(\log s)v_5(s) + (\log s)^2 v_6(s)\right| < 3.7. \tag{3.96}$$

(2) *We have upper bounds for $u_j(z)/z$ and $v_j(z)/z$ as given in the following table:*

	$j =$	3	4	5	6	7	8
$z \in S_{5/27}$	$\lvert u_j(z)/z\rvert <$	1.3	1.409				
$z \in S_{10/27}$	$\lvert u_j(z)/z\rvert <$	1.44	1.721				
	$\lvert v_j(z)/z\rvert <$	1.01	1.02	2.09	5.46	19.1	73

Proof: The inequalities ((3.88)) are inequalities for rational functions and therefore are straightforward to prove using standard methods from classical analysis (or by the use of CAD; see Footnote 9). For the inequalities ((3.89))–((3.96)), we apply a numerical approach (analogous to the one in the proof of Lemma 3.A.3 below). Let $\mathrm{LHS}(s)$ denote the left-hand side of one such inequality. We choose $M = 10^6$ equally spaced points in the interval $[0, 1]$. Then we have

$$\sup_{s\in[0,1]} \mathrm{LHS}(s) \leqslant \sup_{0\leqslant m\leqslant M} \mathrm{LHS}\left(\frac{m}{M}\right) + \frac{1}{M} \sup_{s\in[0,1]} \left|\frac{d\,\mathrm{LHS}}{ds}(s)\right|.$$

The supremum of the derivative can easily be bounded since it is a rational function in s and $\log s$ that has a finite value at $s = 0$.

For the inequalities in Part (2) of the lemma, we also apply this numerical approach. This is indeed feasible since, by the maximum modulus principle, the maximum modulus of an analytic function on a compact domain (which, in our case, are the sets $S_{5/27}$ respectively $S_{10/27}$) is attained at the boundary of the domain. □

3.A.2 Bounds for certain truncated perturbed Gaußian integrals

The central result of this subsection is Lemma 3.A.3 which provides estimates for the constants that appear in Lemma 3.8.1, and which are used in Lemma 3.8.3. A simple corollary of the lemma that is used in the proof of Lemma 3.8.1 is stated separately as Corollary 3.A.4. The lemma below gives an estimate involving the lower incomplete gamma function that is needed in the proof of Lemma 3.A.3.

Below, we will occasionally make use of the effective form of Stirling's formula

$$\Gamma(x) = \left(\frac{x}{e}\right)^x \frac{(2\pi)^{1/2}}{x^{1/2}} e^{\sigma(x)}, \qquad x > 0, \tag{3.97}$$

where

$$0 < \sigma(x) < \frac{1}{12x}.$$

Here, the left inequality follows from [**AnARAA**], while the right inequality follows from [**AnARAA**].

Lemma 3.A.2 *Let $\gamma(s,a) := \int_0^a e^{-x}x^{s-1}dx$ be the lower incomplete gamma function. Suppose that $c, d, \mu \in \mathbb{R}^+$ with $d > c$. Then we have*

$$\sup_{w\in\mathbb{R}^+} w^{-c}\gamma(d,\mu w) \leqslant \frac{\mu^c\Gamma(d-c+1)}{c\sqrt{2\pi(d-c)}}.$$

Proof: We note that the limit of $w^{-c}\gamma(d,\mu w)$ is 0 for both $w \to 0^+$ (here we use that $d > c$) and $w \to +\infty$. This implies that the maximum value of $w^{-c}\gamma(d,\mu w)$ with $w \in \mathbb{R}^+$ occurs at a point where $\frac{d}{dw}(w^{-c}\gamma(d,\mu w)) = 0$. It is straightforward to see that this latter equation is equivalent to

$$\gamma(d,\mu w) = \frac{e^{-\mu w}(\mu w)^d}{c}.$$

Therefore, we have

$$\sup_{w\in\mathbb{R}^+} w^{-c}\gamma(d,\mu w) \leqslant \sup_{w\in\mathbb{R}^+} \frac{e^{-\mu w}w^{d-c}\mu^d}{c}.$$

Another differentiation shows that the supremum of the latter expression occurs at $w = (d-c)/\mu$, which gives a final bound of

$$\sup_{w\in\mathbb{R}^+} w^{-c}\gamma(d,\mu w) \leqslant \frac{\mu^c e^{-(d-c)}(d-c)^{d-c}}{c} < \frac{\mu^c\Gamma(d-c+1)}{c\sqrt{2\pi(d-c)}},$$

where, to get the last bound, we used the lower bound in ((3.97)). This is exactly what we wanted to prove. □

Lemma 3.A.3 *There exist functions $\beta_i : (0,1) \to \mathbb{R}^+$ for $i = 1,2,3,4$, defined by*

$$\beta_1(\mu) := \sup_{w>0} \frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})} \int_0^\mu e^{-wy^2}\left(\cosh(wy^3) - 1\right) dy, \tag{3.98}$$

$$\beta_2(\mu) := \sup_{w>0} \frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})} \int_0^\mu ye^{-wy^2}\sinh(wy^3)\, dy, \tag{3.99}$$

$$\beta_3(\mu) := \sup_{w>0} \frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})} \int_0^\mu e^{-wy^2}\sinh(wy^4)\, dy, \tag{3.100}$$

$$\beta_4(\mu) := \sup_{w>0} \frac{w^{2}}{\operatorname{erf}(\mu\sqrt{w})} \int_0^\mu ye^{-wy^2}\sinh(wy^4)\, dy. \tag{3.101}$$

Moreover, we have the following estimates for particular values:

$$\beta_1(20/27) < 1.39, \qquad \beta_2(20/27) < 1.14, \qquad \beta_3(2/3) < 0.73, \qquad \beta_4(2/3) < 1.15.$$

Proof: We provide here only the proof concerning β_1. The proofs for the other three suprema are completely analogous.

We must first show that the supremum in ((3.98)) is always finite. Let

$$b_1(\mu,w) := \frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})} \int_0^\mu e^{-wy^2}\left(\cosh(wy^3) - 1\right) dy$$

abbreviate the function of which we want to take the supremum. We first note that the integrand in the above integral is bounded above by $\exp(-wy^2(1-y))$ and therefore also by 1. Hence,

$$b_1(\mu, w) \leqslant \frac{\mu w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})}.$$

On the other hand, we perform a Taylor expansion of $\cosh(wx^3) - 1$, and define

$$u_1(k, \mu, w) := \frac{w^{3/2}}{(2k)!} \int_0^\mu e^{-wy^2} w^{2k} y^{6k}\, dy = \frac{\gamma(3k + 1/2, \mu^2 w)}{2(2k)!\, w^{k-1}},$$

so that

$$b_1(\mu, w) = \frac{1}{\operatorname{erf}(\mu\sqrt{w})} \sum_{k=1}^{\infty} u_1(k, \mu, w).$$

Now, Lemma 3.A.2 implies that

$$u_1(k, \mu, w) < \frac{\mu^{2k-2}\Gamma(2k + 5/2)}{2(2k)!\,(k-1)\sqrt{(4k+3)\pi}} < \frac{(k+1)}{(k-1)\sqrt{2\pi}}\mu^{2k-2},$$

where we used ((3.97)) to obtain the last inequality. On the other hand, we trivially have

$$u_1(k, \mu, w) < \frac{\Gamma(3k + 1/2)}{2(2k)! w^{k-1}}.$$

Both bounds combined, we find

$$b_1(\mu, w) \leqslant \frac{1}{\operatorname{erf}(\mu\sqrt{w})} \min\left(\mu w^{3/2}, \frac{\Gamma(7/2)}{4} + \frac{\Gamma(13/2)}{48w} + \frac{1}{\sqrt{2\pi}} \sum_{k=3}^{\infty} \frac{k+1}{k-1}\mu^{2k-2}\right).$$

This confirms the finiteness of the supremum in ((3.98)) and therefore the existence of the function β_1.

In order to determine the particular value $\beta_1(20/27)$ (at least approximately), we first dispose of large w by providing an upper bound for $b_1(20/27, w)$ for $w > w_0 := 80$. Indeed, in this regime we have $\mu\sqrt{w} > 6$, and therefore

$$b_1(20/27, w) < \frac{1}{\operatorname{erf} 6}\left(\frac{\Gamma(7/2)}{4} + \frac{\Gamma(13/2)}{48w_0} + \frac{1}{\sqrt{2\pi}} \sum_{k=3}^{\infty} \frac{k+1}{k-1}(20/27)^{2k-2}\right) < 1.37.$$

We then determine the supremum of $b_1(20/27, w)$ over the interval $[0, w_0]$ by a routine calculation. Namely, to begin with, we provide a crude upper bound for the derivative $\frac{\partial b_1}{\partial w}(\mu, w)$ in this interval. To this end, we argue that the inequality $\operatorname{erf}(x) > x/(1+x)$ implies that

$$\frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})} < \frac{w(1 + \mu\sqrt{w})}{\mu}$$

and

$$\begin{aligned}\left|\frac{\partial}{\partial w}\frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})}\right| &= \left|\frac{3\sqrt{w}}{2\operatorname{erf}(\mu\sqrt{w})} - \frac{\mu w e^{-\mu^2 w}}{\sqrt{\pi}\operatorname{erf}^2(\mu\sqrt{w})}\right| \\ &\leqslant \frac{3\sqrt{w}}{2\operatorname{erf}(\mu\sqrt{w})} + \frac{\mu w e^{-\mu^2 w}}{\sqrt{\pi}\operatorname{erf}^2(\mu\sqrt{w})} \\ &< \frac{3(1+\mu\sqrt{w})}{2\mu} + \frac{(1+\mu\sqrt{w})^2}{\mu\sqrt{\pi}} < \frac{4(1+\mu\sqrt{w})^2}{\mu\sqrt{\pi}}.\end{aligned}$$

On the other hand, for all $y \in [0,\mu]$ we have

$$e^{-wy^2}\left(\cosh(wy^3)-1\right) < e^{-wy^2+wy^3} \leqslant 1,$$

and

$$\begin{aligned}\left|\frac{\partial}{\partial w}e^{-wy^2}\left(\cosh(wy^3)-1\right)\right| &= \left|y^2 e^{-wy^2}(y\sinh(wy^3)-\cosh(wy^3)+1)\right| \\ &< y^2 e^{-wy^2+wy^3} \leqslant \mu^2.\end{aligned}$$

Combining these inequalities, we obtain

$$\begin{aligned}\left|\frac{\partial b_1}{\partial w}(\mu,w)\right| &\leqslant \left|\frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})}\int_0^\mu \frac{\partial}{\partial w}\left(e^{-wy^2}\left(\cosh(wy^3)-1\right)\right)dy\right| \\ &\quad + \left|\left(\frac{\partial}{\partial w}\frac{w^{3/2}}{\operatorname{erf}(\mu\sqrt{w})}\right)\int_0^\mu e^{-wy^2}\left(\cosh(wy^3)-1\right)dy\right| \\ &\leqslant (\mu^2)w(1+\mu\sqrt{w}) + \frac{4(1+\mu\sqrt{w})^2}{\sqrt{\pi}} < \frac{6}{\sqrt{\pi}}w_0(1+\mu\sqrt{w_0})^2.\end{aligned}$$

With this upper bound proven, we choose $M = 10^6$ uniformly distributed points in the interval $[0, w_0]$, and argue that

$$\sup_{w\in[0,w_0]} b_1(20/27,w) \leqslant \sup_{0\leqslant m\leqslant M} b_1\left(20/27, \frac{m}{M}w_0\right) + \frac{w_0}{M}\sup_{w\in[0,w_0]}\left|\frac{\partial b_1}{\partial w}(20/27,w)\right|.$$

The result of this calculation turns out to be $1.3860 < 1.39$ (accurate to the last significant digit given), which finishes the proof. □

Corollary 3.A.4 *For $u, v \in \mathbb{R}^+$ and $x_0 \in [0, u/v]$, we have*

$$\int_0^{x_0} e^{-ux^2}\left(\cosh(vx^3)-1\right)dx \leqslant \beta_1\left(x_0\frac{v}{u}\right)\frac{v^2}{u^{7/2}}\operatorname{erf}(x_0\sqrt{u}), \tag{3.102}$$

$$\int_0^{x_0} xe^{-ux^2}\sinh(vx^3)\,dx \leqslant \beta_2\left(x_0\frac{v}{u}\right)\frac{v}{u^{5/2}}\operatorname{erf}(x_0\sqrt{u}), \tag{3.103}$$

$$\int_0^{x_0} e^{-ux^2}\sinh(vx^4)\,dx \leqslant \beta_3\left(x_0\sqrt{\frac{v}{u}}\right)\frac{v}{u^{5/2}}\operatorname{erf}(x_0\sqrt{u}), \tag{3.104}$$

$$\int_0^{x_0} xe^{-ux^2} \sinh(vx^4)\, dx \leqslant \beta_4\left(x_0\sqrt{\frac{v}{u}}\right)\frac{v}{u^3}\operatorname{erf}(x_0\sqrt{u}). \tag{3.105}$$

Proof: This follows immediately from Lemma 3.A.3 by, on the one hand, performing the substitutions $y \to (v/u)x$ and $w \to u^3/v^2$ in ((3.98)) and ((3.99)), and performing the substitutions $y \to (\sqrt{v/u})x$ and $w \to u^2/v$ in ((3.100)) and ((3.101)). □

3.A.3 A Maclaurin summation estimate

The following upper bound for an alternating sum is crucial in the proof of Lemma 3.8.2, see ((3.46)).

Lemma 3.A.5 *For $n \in \mathbb{Z}^+$ and $f \in C^4[0, 3n]$, we have*

$$\left|\sum_{k=1}^{n}(f(3k-2)-f(3k-1))\right| \leqslant \frac{1}{3}\left|f(3n)-f(0)\right| + \frac{2}{3}\left|f''(3n)-f''(0)\right| + \frac{11}{96}\sup_{x\in[0,3n]}|f^{(4)}(x)|.$$

Proof: We use the offset Maclaurin summation formula (see, for example, [Sid03, Theorem D.2.4]) to see that

$$\begin{aligned}\sum_{k=1}^{n}(f(3k-2)-f(3k-1)) &= \sum_{k=1}^{4}\frac{3^{k-1}(B_k(2/3)-B_k(1/3))}{k!}\left(f^{(k-1)}(3n)-f^{(k-1)}(0)\right)\\ &\quad -\frac{9}{8}\int_0^{3n} f^{(4)}(x)\left(\bar{B}_4\left(\frac{2-x}{3}\right)-\bar{B}_4\left(\frac{1-x}{3}\right)\right)dx\\ &= \frac{1}{3}\left(f(3n)-f(0)\right)-\frac{2}{3}\left(f''(3n)-f''(0)\right)\\ &\quad -\frac{9}{8}\int_0^{3n} f^{(4)}(x)\left(\bar{B}_4\left(\frac{2-x}{3}\right)-\bar{B}_4\left(\frac{1-x}{3}\right)\right)dx,\end{aligned}$$

where the Bernoulli polynomials $B_k(u)$ are defined by

$$\sum_{k\geqslant 0} B_k(u)\frac{t^k}{k!} = \frac{te^{ut}}{e^t-1},$$

and $\bar{B}_k(u) = B_k(\{u\})$, with $\{u\}$ denoting the fractional part of u as usual, is the k-th periodic Bernoulli function. The lemma follows from the fact that

$$\int_0^{3n}\left|\bar{B}_4\left(\frac{2-x}{3}\right)-\bar{B}_4\left(\frac{1-x}{3}\right)\right|dx = \frac{11n}{108}.$$

□

3.A.4 Estimates for sums and differences of exponentials

Here we record two elementary estimates for the difference respectively the sum of two exponentials that are used in the proof of Lemma 3.8.1.

Lemma 3.A.6 *For $z, w \in \mathbb{C}$, we have the following inequalities:*

$$|e^z - e^w| \leqslant 2\sinh\max(|z|,|w|) + 2\sinh\frac{|z+w|}{2}, \tag{3.106}$$

$$|e^z + e^w - 2| \leqslant 2\cosh\max(|z|,|w|) - 2 + 2\sinh\frac{|z+w|}{2}. \tag{3.107}$$

Proof: Without loss of generality, we assume that $\mathrm{Re}(w-z) \leqslant 0$. By the triangle inequality, we have

$$\begin{aligned}|e^z - e^w| &\leqslant \left|e^z - e^{-z}\right| + \left|e^{-z} - e^w\right| \\ &\leqslant 2\sinh|z| + 2\left|e^{(w-z)/2}\right|\sinh\frac{|z+w|}{2} \\ &\leqslant 2\sinh\max(|z|,|w|) + 2\sinh\frac{|z+w|}{2},\end{aligned}$$

and

$$\begin{aligned}|e^z + e^w - 2| &\leqslant \left|e^z + e^{-z} - 2\right| + \left|e^{-z} - e^w\right| \\ &\leqslant 2\cosh|z| - 2 + 2\left|e^{(w-z)/2}\right|\sinh\frac{|z+w|}{2} \\ &\leqslant 2\cosh\max(|z|,|w|) - 2 + 2\sinh\frac{|z+w|}{2}.\end{aligned}$$

□

3.A.5 Inequalities for the sums $X_j(n,r)$

The lemma below provides inequalities for various expressions involving the sums $X_j(n,r)$ defined in ((3.18)). These are used in the proof of Lemma 3.8.2 and for the proof of several particular bounds presented in Corollary 3.A.8 below. In their turn, the bounds of the corollary are used in Lemmas 3.8.3 and 3.9.4.

Lemma 3.A.7 *For $n \in \mathbb{Z}^+$ and $r \in (0,1]$, we have the following inequalities concerning the quantities $X_j(n,r)$:*

1. $$X_1(n,r) \geqslant \frac{r(1+2r+2r^3+r^4)(1-r^{3n})(1-r^{3n/2})}{(1-r^3)^2}. \tag{3.108}$$

2. *For $j = 0,1,2,3$, we have*

$$\frac{X_{j+1}(n,r)}{X_0(n,r)X_j(n,r)} \leqslant \frac{X_{j+1}(\infty,r)}{X_0(\infty,r)X_j(\infty,r)}. \tag{3.109}$$

3. *For $j = 0,1,2$, we have*

$$\frac{X_j(n,r)X_{j+2}(n,r)}{X_{j+1}^2(n,r)} \leqslant \frac{X_j(\infty,r)X_{j+2}(\infty,r)}{X_{j+1}^2(\infty,r)}. \tag{3.110}$$

Proof: (1) Inequality ((3.108)) can be proved by observing that

$$\begin{aligned}
X_1(n,r)(1-r^3)^2 &= r(1+2r+2r^3+r^4)(1-r^{3n}) - 3nr^{3n+1}(1+r)(1-r^3)\\
&\geqslant r(1+2r+2r^3+r^4)(1-r^{3n}) - r^{3n/2+1}(3r^{3/2}+3r^{5/2})(1-r^{3n})\\
&\geqslant r(1+2r+2r^3+r^4)(1-r^{3n}) - r^{3n/2+1}(1+2r+2r^3+r^4)(1-r^{3n})\\
&= r(1+2r+2r^3+r^4)(1-r^{3n})(1-r^{3n/2}).
\end{aligned}$$

(2) To prove ((3.109)) and ((3.110)), we claim that the expressions

$$\frac{(1-r^3)^{j+2}}{(1+r)r^{3n+3}}\left(X_{j+1}(\infty,r)X_0(n,r)X_j(n,r) - X_{j+1}(n,r)X_0(\infty,r)X_j(\infty,r)\right)$$

and

$$\frac{(1-r^3)^{2j+4}}{3nr^{3n+4}}\left(X_j(\infty,r)X_{j+2}(\infty,r)X_{j+1}^2(n,r) - X_j(n,r)X_{j+2}(n,r)X_{j+1}^2(\infty,r)\right)$$

are actually polynomials in r with non-negative coefficients. This claim can be routinely verified by explicitly calculating each coefficient of these expressions as piecewise polynomial function. As an illustrative example, we have

$$\frac{(1-r^3)^4}{3nr^{3n+4}}\left(X_0(\infty,r)X_2(\infty,r)X_1^2(n,r) - X_0(n,r)X_2(n,r)X_1^2(\infty,r)\right) = (1+r)\sum_{m=0}^{3n+2} a_m r^m,$$

where the coefficients are given by $a_0 = 3n$, $a_1 = 15n-2$, $a_2 = 24n-4$, $a_3 = 30n-18$, $a_{3n} = 27n-18$, $a_{3n+1} = 3n-4$, $a_{3n+2} = 3n-2$, and

$$a_m = \begin{cases} 3(2m-3)(3n-m)+9(m-2), & \text{if } m \equiv 0 \pmod 3,\\ 3(3m-4)(3n-m)+9(m-2), & \text{if } m \equiv 1 \pmod 3,\\ 3(3m-5)(3n-m)+18(m-2), & \text{if } m \equiv 2 \pmod 3. \end{cases}$$

for $4 \leqslant m \leqslant 3n-1$. □

Corollary 3.A.8 *For $n \geqslant 1$ and $r \in (0,1]$, we have*

$$\frac{X_0^2(n,r)}{rX_1(n,r)} \leqslant \frac{4}{3}, \tag{3.111}$$

$$\frac{rX_2(n,r)}{X_0(n,r)X_1(n,r)} \leqslant 3, \tag{3.112}$$

$$\frac{r^2X_2(n,r)}{X_0^3(n,r)} \leqslant \frac{9}{2}, \tag{3.113}$$

$$\frac{rX_3(n,r)}{X_0(n,r)X_2(n,r)} \leqslant \frac{9}{2}, \tag{3.114}$$

$$\frac{r^2X_4(n,r)}{X_0^2(n,r)X_2(n,r)} \leqslant 27, \tag{3.115}$$

$$\frac{X_0(n,r)X_3(n,r)}{X_1(n,r)X_2(n,r)} \leqslant 3, \tag{3.116}$$

$$\frac{X_0(n,r)X_3^2(n,r)}{X_2^3(n,r)} \leqslant \frac{9}{2}, \tag{3.117}$$

$$\frac{X_0(n,r)X_4(n,r)}{X_2^2(n,r)} \leqslant 6, \tag{3.118}$$

where the $X_j(n,r)$ are defined in ((3.18)).

Proof: To prove ((3.111)), we argue that

$$4rX_1(n,r) - 3X_0^2(n,r) = r^2(1-r)(1+3r) \geqslant 0$$

for $n = 1$, and make use of ((3.108)) to see that

$$\frac{X_0^2(n,r)}{rX_1(n,r)} \leqslant \frac{(1+r)^2(1+r^{3n/2})}{(1+2r+2r^3+r^4)} \leqslant \frac{(1+r)^2(1+r^3)}{(1+2r+2r^3+r^4)} \leqslant \frac{4}{3}$$

for $n \geqslant 2$.

For the other seven inequalities, we invoke ((3.109)) for ((3.112))–((3.115)) and ((3.110)) for ((3.116))–((3.118)) to see that the left-hand side of all six inequalities does not exceed the corresponding $n \to \infty$ limit. The six limits in question are simple rational functions in r and can be routinely shown to be bounded above by the right-hand side; as an example, for ((3.113)) we have

$$\frac{r^2X_2(n,r)}{X_0^3(n,r)} \leqslant \frac{r^2X_2(\infty,r)}{X_0^3(\infty,r)} = \frac{1+3r-3r^2+16r^3-3r^4+3r^5-r^6}{(1+r)^2},$$

and

$$9(1+r)^2 - 2(1+3r-3r^2+16r^3-3r^4+3r^5-r^6) = (1-r)(7+19r+34r^2+2r^3+8r^4+2r^5) \geqslant 0.$$

□

3.A.6 Upper bounds for certain trigonometric sums

This subsection contains two auxiliary results, of different flavour, which provide upper bounds for the absolute value of certain trigonometric sums, the second more special than the first. Lemma 3.A.9 is used in the proofs of Lemmas 3.9.1 and 3.9.3, while Lemma 3.A.10 is used in the proof of Lemma 3.9.2. An auxiliary result that is needed in the proof of Lemma 3.A.10 is stated separately in Lemma 3.A.11.

Lemma 3.A.9 *Suppose that $0 < r \leqslant 1$ and $\theta, \varphi \in \mathbb{R}$. For all positive monotonically increasing sequences $\{u_n\}_{n\geqslant 0}$, and for all non-negative integers a, b such that $a \leqslant b$, we have*

$$\left|\sum_{k=a}^{b} u_k r^k \cos(k\theta+\varphi)\right| \leqslant \frac{1}{|1-re^{i\theta}|}\left((1-r)\sum_{k=a}^{b} u_k r^k + 2r^{b+1}u_b\right).$$

Proof: We write $z = re^{i\theta}$, and note that the sum $S_{a,b} := \sum_{k=a}^{b} r^k \cos(k\theta+\varphi)$ can be bounded above by

$$\left|\sum_{k=a}^{b} r^k \cos(k\theta+\varphi)\right| \leqslant \left|\sum_{k=a}^{b} z^k\right| = \left|\frac{z^a - z^{b+1}}{1-z}\right| \leqslant \frac{r^a + r^{b+1}}{|1-z|}.$$

Therefore, we can use Abel's lemma (summation by parts) to get

$$\begin{aligned}\left|\sum_{k=a}^{b} u_k r^k \cos(k\theta+\varphi)\right| &\leqslant u_a|S_{a,b}| + (u_{a+1}-u_a)|S_{a+1,b}| + \cdots + (u_b - u_{b-1})|S_{b,b}| \\ &\leqslant \frac{1}{|1-z|}\Big(u_a(r^a + r^{b+1}) + (u_{a+1}-u_a)(r^{a+1}+r^{b+1}) + \cdots + (u_b-u_{b-1})(r^b + r^{b+1})\Big) \\ &= \frac{1}{|1-z|}\left((1-r)\sum_{k=a}^{b} u_k r^k + 2r^{b+1}u_b\right). \qquad \square\end{aligned}$$

The following inequality improves Lemma B.4 from [Wan22].

Lemma 3.A.10 *For $r \in (0,1)$, $n \in \mathbb{Z}^+$, and $\theta \in [-\pi,\pi]$, we have*

$$\sum_{k=1}^{n} r^{k-1}\cos k\theta \leqslant \frac{1-r^n}{1-r}\sqrt{\frac{1}{1+4\kappa\tan^2(\theta/2)}}, \tag{3.119}$$

where

$$\kappa = \frac{(1+r)(1-r^n)(1-r^{n/6})}{(1-r)^2}.$$

Proof: Writing $\cos(k\theta) = \frac{1}{2}\left(e^{ik\theta} + e^{-ik\theta}\right)$, we see that the sum on the left-hand side can be evaluated as it is just the sum of two geometric series. After substitution of the result, it turns out that the claimed inequality is equivalent to

$$\frac{-r+\cos\theta + r^{n+1}\cos(n\theta) - r^n\cos(n\theta+\theta)}{1-2r\cos\theta+r^2} \leqslant \frac{1-r^n}{1-r}\sqrt{\frac{1}{1+4\kappa\tan^2(\theta/2)}}. \tag{3.120}$$

Without loss of generality we assume that $\theta \geqslant 0$. We prove ((3.120)) for all *real* $n \geqslant 1$ and $\theta \in [0,\pi]$. We divide the proof into two parts according to whether θ is larger than $\frac{\pi}{n+1}$ or not.

PART I. $\theta \leqslant \frac{\pi}{n+1}$. We construct Padé approximants as bounds for the various non-rational functions involved, with the goal of reducing the proof of the inequality to the proof of an inequality for a *rational function*. The reason is that inequalities for rational functions are easier to handle. In particular, they can be automatically proved by using *Cylindrical Algebraic Decomposition* (CAD),[9] and this is what we are going to do in the end for the most intricate ones.

We let $t = \tan^2(\theta/2)$ so that $\cos\theta = \frac{1-t}{1+t}$. Using Lemma 3.A.11 below, Lemma B.3 from [Wan22], and elementary manipulations, we obtain

$$\cos(n\theta) = \frac{3+(3-5n^2)t - n^2t^2}{(1+t)(3+n^2t)} \geqslant \frac{3-(5n^2-2)t}{3+(n^2+2)t}, \quad \text{for all } \theta \in \mathbb{R},$$

[9] Cylindrical Algebraic Decomposition (CAD) is an algorithm that, among others, is able to *prove* that a given polynomial in several variables is positive (non-negative), respectively provides a description of the subset of the parameter space for which the polynomial is positive (non-negative). It also allows one to verify the positivity (non-negativity) of polynomials in several variables under (polynomial) constraints on the variables. The reader is referred to the "user guide" [**MR2773014**] and the references therein. Implementations of CAD are available within any standard computer algebra programme. The one that we used is the command `CylindricalDecomposition` within *Mathematica*.

$$\cos(n\theta) - \cos(n\theta + \theta) \leqslant \frac{6(2n+1)t}{3 + (2n^2 + 2n + 3)t}, \quad \text{for all } \theta \in [0, \pi/n],$$
$$\frac{1}{\sqrt{1+4x}} \geqslant \frac{1}{1+2x}, \quad \text{for all } x \geqslant 0.$$

With these inequalities in mind, it is sufficient to prove that

$$(1-r)\left(1 - r^n \frac{3 - (5n^2-2)t}{3 + (n^2+2)t}\right) - 1 + \frac{1-t}{1+t} + r^n \frac{6(2n+1)t}{3 + (2n^2+2n+3)t}$$
$$\leqslant \frac{1-r^n}{1-r}\left(1 - 2r\frac{1-t}{1+t} + r^2\right)\frac{1}{1+2\kappa t}. \tag{3.121}$$

The difference between the two sides of ((3.121)) can be written as

$$\frac{2t(9a_0 + 3a_1 t + a_2 t^2 + \kappa(1-r)a_3 t^3)}{(1-r)^2(1+t)(3+(n^2+2)t)(3+(2n^2+2n+3)t)(1+2\kappa t)}, \tag{3.122}$$

where

$$\begin{aligned}
a_0 &= 1 + r - r^n\left((1+n(1-r))^2 + r\right) - \kappa(1-r)^2(1-r^n),\\
a_1 &= 2(n^2+n+3)a_0 + 3\kappa(1-r)(1+r-3r^n+r^{n+1})\\
&\quad + (n^2-1)(1+r-2r^{n+1}) + (n+1)^2(2n+1)r^n(1-r)\\
&\quad - \kappa(1-r)\left((n^2-1)(1-r)(1+5r^n) + 12nr^n\right),\\
a_2 &= \sum_{j=0}^{4} a_{2j} n^j, \text{ with}\\
&\quad a_{20} = 3(1-r^n)(2+2r+\kappa(1-r)(3+7r)),\\
&\quad a_{21} = 4(1+r-3r^n+r^{n+1}) + 2\kappa(1-r)(1+5r-25r^n-5r^{n+1})),\\
&\quad a_{22} = 7+7r-12r^n+7r^{n+1}-9r^{n+2} + 2\kappa(1-r)(1+8r-13r^n+10r^{n+1}),\\
&\quad a_{23} = 2(1+r-6r^n+7r^{n+1}-3r^{n+2}) - 2\kappa(1-r)(1-r+11r^n-5r^{n+1}),\\
&\quad a_{24} = 2(1+r-3r^n+4r^{n+1}-6r^{n+2}) - 2\kappa(1-r)^2(1+5r^n),\\
a_3 &= (1+r)(1-r^n)(n^2+2)(2n^2+2n+3)\\
&\quad - 6n^2r^n(1-r)(2n^2+2n+3) + 4nr^n(n-2)(n^2+2).
\end{aligned}$$

In the following, we are going to prove non-negativity results for these coefficients.

(1) $a_0 \geqslant 0$. We substitute the definition of κ in ((3.122)). After some simplification, the inequality can be shown to be equivalent to

$$\frac{(1+n(1-r))^2 + r}{1+r} \leqslant \frac{1-(1-r^n)^2(1-r^{n/6})}{r^n}. \tag{3.123}$$

In order to prove this, we first use the classical inequalities $1-r \leqslant (-\log r)$ and $\frac{1-r}{1+r} \leqslant (-\log r)/2$ to conclude that

$$\frac{(1+n(1-r))^2+r}{1+r} \leqslant 1+(-\log r)n+(-\log r)^2\frac{n^2}{2}.$$

Note that the right-hand side is exactly the Taylor polynomial of

$$r^{-n}(1-(1-r^n)^2(1-r^{n/6}))$$

of order 2 at $n=0$. So, in order to prove ((3.123)), it suffices to show that its third derivative is non-negative. Indeed, this third derivative can be calculated as

$$\begin{aligned}\left(\frac{d}{dn}\right)^3 \frac{(1-(1-r^n)^2(1-r^{n/6}))}{r^n} \\ = \frac{(-\log r)^3 r^{n/6}}{216}\left(125r^{-n}+2+216r^{5n/6}-343r^n\right) \geqslant 0.\end{aligned}$$

(2) $a_1 \geqslant 0$. We claim that

$$\begin{aligned}(n^2-1)(1+r-2r^{n+1})+(n+1)^2(2n+1)r^n(1-r) \\ \geqslant \kappa(1-r)^2(n^2-1)(1+5r^n)+12n\kappa r^n(1-r). \quad (3.124)\end{aligned}$$

By substituting the definition of κ and using the inequality $1+5r^n \leqslant (1-r^n)/(1-r^{n/6})$, we see that ((3.124)) is implied by

$$2n(n+1)(n+2) \geqslant \frac{1-r^n}{1-r}(1+r)\left(12n\frac{1-r^{n/6}}{1-r}-n^2+1\right).$$

This can be proved by noting that $n \geqslant (1-r^n)/(1-r)$, and that

$$\begin{aligned}(1+r)\left(12n\frac{1-r^{n/6}}{1-r}-n^2+1\right) &\leqslant \begin{cases}(1+r)\left(2n^2-n^2+1\right), & \text{if } n \geqslant 6,\\ 12n\frac{1-r^{n/6}}{1-\sqrt{r}}-n^2+1, & \text{if } n<6,\end{cases}\\ &\leqslant \begin{cases}2n^2+2, & \text{if } n \geqslant 6,\\ 12n\max(1,n/3)-n^2+1, & \text{if } n<6,\end{cases}\\ &< 2(n+1)(n+2).\end{aligned}$$

(3) $a_2 \geqslant 0$. We prove that a_{20}, a_{22}, a_{24}, $(1-r^{1/6})a_{21}+(1-r^{n/6})a_{22}$ and $\sum_{j=0}^{4}(1-r^{1/6})^{4-j}(1-r^{n/6})^j a_{2j}$ are non-negative. All these expressions are rational functions in $r^{1/6}$ and $r^{n/6}$. In order to get these expressions ready for application of CAD, we replace each occurrence of $r^{n/6}$ by X, and each occurrence of $r^{1/6}$ by Y, say. In this manner, we obtain rational functions in X and Y. (In order to illustrate this: a term $r^{n+2/3}$ would be replaced by X^6Y^2.) Now CAD can be applied under the constraints $0<X \leqslant Y<1$, and it yields the claimed result.

(4) $(1-r^{n/6})a_2+\kappa(1-r)(1-r^{1/6})a_3 \geqslant 0$. The proof is completely analogous to the proof of $a_2 \geqslant 0$ above: we write

$$(1-r^{n/6})a_2+\kappa(1-r)(1-r^{1/6})a_3 = \sum_{j=0}^{4} n^j b_j,$$

and verify by CAD that $b_0, b_2, b_4, (1-r^{1/6})b_1+(1-r^{n/6})b_2$ and

$$\sum_{j=0}^{4}(1-r^{1/6})^{4-j}(1-r^{n/6})^j b_j$$

are non-negative.

With these non-negativity results proven, the inequality ((3.121)) follows from the fact that

$$t \leqslant \tan^2\left(\frac{\pi}{2n+2}\right) \leqslant \frac{1}{n} \leqslant \frac{1-r^{1/6}}{1-r^{n/6}}.$$

PART II. $\theta > \frac{\pi}{n+1}$. We apply the Cauchy–Schwarz inequality to the vectors $(r-\cos\theta, \sin\theta)$ and $(\cos n\theta, \sin n\theta)$. This yields

$$(r-\cos\theta)\cos n\theta + \sin\theta \sin n\theta \leqslant \sqrt{(r-\cos\theta)^2+\sin^2\theta}\cdot 1,$$

which is equivalent to

$$r\cos(n\theta) - \cos(n\theta+\theta) \leqslant \sqrt{1-2r\cos\theta+r^2}. \tag{3.125}$$

Equality in ((3.125)) holds if and only if the two vectors are proportional to each other, that is, if and only if

$$\frac{r-\cos\theta}{\sin\theta} = \frac{\cos n\theta}{\sin n\theta} = \cot n\theta.$$

We define the quantity

$$n_0(\theta, r) = \frac{1}{\theta}\left(\frac{\pi}{2} - \arctan\frac{r-\cos\theta}{\sin\theta}\right) \in \left[\frac{\pi-\theta}{2\theta}, \frac{\pi-\theta}{\theta}\right].$$

From the above observation, it follows readily that we have equality in ((3.125)) for $n = n_0(\theta, r)$.

We now claim that the strengthened inequality

$$\frac{-r+\cos\theta+s\sqrt{1-2r\cos\theta+r^2}}{1-2r\cos\theta+r^2} \leqslant \frac{1-s}{1-r}\sqrt{\frac{1}{1+4\kappa^*\tan^2(\theta/2)}}, \tag{3.126}$$

holds in the region

$$\left\{(r,s,\theta) : r,s \in [0,1),\ 0 \leqslant \theta < \pi,\ s \leqslant r^{\max(1,n_0(\theta,r))}\right\},$$

where κ^* is defined by

$$\kappa^* := \frac{(1+r)(1-s)(1-s^{1/6})}{(1-r)^2}.$$

If we assume the validity of this inequality, then the desired result follows by choosing $s = r^n$ in ((3.126)), and applying ((3.125)); we point out that, since $n_0(\theta, r) \leqslant \pi/\theta - 1 < n$, our desired value of $s = r^n$ indeed belongs to the region.

In order to prove ((3.126)), first note that the left-hand side of ((3.126)) is linear with respect to s. Furthermore, computation of the second derivative of the right-hand side shows that it is concave with respect to s. Therefore it suffices to prove ((3.126)) for the values of s on the boundary — that is, for $s = 0$ and $s = r^{\max(1, n_0(\theta, r))}$. We write $c := \cos\theta$ for simplicity of notation.

(1) $s = 0$. In this case, the inequality ((3.126)) reduces to

$$\frac{c-r}{1-2rc+r^2} \leqslant \sqrt{\frac{1}{(1-r)^2 + 4(1+r)\frac{1-c}{1+c}}}.$$

This inequality clearly holds if $c \leqslant r$. If $r < c \leqslant 1$, then we have

$$\frac{1}{(1-r)^2 + 4(1+r)\frac{1-c}{1+c}} - \frac{(c-r)^2}{(1-2cr+r^2)^2}$$
$$= \frac{(1-c)^2(1+r)^2(1+3c-2r)}{(1-2cr+r^2)^2((1-c)(1+r)(5-r)+2(c-r)(1-r))} \geqslant 0.$$

(2) $s = r$ AND $n_0(\theta, r) \leqslant 1$. Elementary manipulations reveal that the inequality for n_0 is equivalent to $r \geqslant 2c$. Moreover, the equality $s = r$ implies that

$$\kappa = \frac{(1+r)(1-r^{1/6})}{1-r} \leqslant \frac{1+r}{1+\sqrt{r}} \leqslant 1.$$

So it suffices to prove that

$$\frac{c - r + r\sqrt{1-2rc+r^2}}{1-2rc+r^2} \leqslant \sqrt{\frac{1}{1+4\frac{1-c}{1+c}}} = \sqrt{\frac{1+c}{5-3c}} \tag{3.127}$$

holds for $r \in [0,1]$ and $c \in [-1, r/2]$. We argue that the left-hand side of ((3.127)) is increasing with respect to r for $r \in [\max(0, 2c), 1]$ because of

$$\frac{\partial}{\partial r}\frac{c - r + r\sqrt{1-2rc+r^2}}{1-2rc+r^2} = \frac{(1-cr)\sqrt{1-2cr+r^2} - (1-c^2-(r-c)^2)}{(1-2cr+r^2)^2},$$

and that

$$(1-cr)^2(1-2cr+r^2) - (1-c^2-(r-c)^2)^2 = (1-c^2)(r-2c)(3r-2c-r^3) \geqslant 0.$$

Therefore we have

$$\frac{c - r + r\sqrt{1 - 2rc + r^2}}{1 - 2rc + r^2} \leqslant \frac{1}{\sqrt{2 - 2c}} - \frac{1}{2} \leqslant \frac{1 + c}{3} \leqslant \sqrt{\frac{1 + c}{5 - 3c}},$$

as desired.

(3) $s = r^{n_0(\theta,r)}$ AND $n_0(\theta, r) \geqslant 1$. We recall that ((3.125)) holds for $n = n_0(\theta, r)$. This means that ((3.126)) is equivalent to the special case of ((3.120)) where n is replaced by $n_0(r, \theta)$. Since we have $n_0 \leqslant \pi/\theta - 1$ and therefore $\theta \leqslant \pi/(n_0 + 1)$, we invoke the result of the first part to conclude the proof. □

The following inequality proves that a Padé approximant of $\cos(n\theta) - \cos(n\theta + \theta)$ is a lower bound in a small interval around 0.

Lemma 3.A.11 *For $n \geqslant 1$ and $\theta \in [-\pi/n, \pi/n]$, we have*

$$\cos(n\theta) - \cos(n\theta + \theta) \leqslant \frac{6(2n + 1)}{3\cot^2(\theta/2) + 2n^2 + 2n + 3}. \tag{3.128}$$

Proof: Without loss of generality assume that $\theta \in [0, \pi/n]$. If $\theta > 2\pi/(2n+1)$ then the left-hand side of ((3.128)) is negative and there is nothing to prove. Otherwise let $\phi := (2n+1)\theta/2 \in [0, \pi]$ and $m := 2n+1$. By elementary manipulations, we see that the inequality ((3.128)) is equivalent to

$$m \sin\frac{\phi}{m} \geqslant \left(1 + \frac{m^2 - 1}{6}\sin^2\frac{\phi}{m}\right)\sin\phi.$$

We use the fact that $\sin^2(\phi/m) \leqslant (\phi/m)^2$ to observe that it suffices to prove

$$m \sin\frac{\phi}{m} \geqslant \left(1 + \frac{m^2 - 1}{6m^2}\phi^2\right)\sin\phi.$$

This is evidently an equality if $m = 1$. We claim that the difference between the two sides is increasing with respect to m. Indeed, we have

$$\begin{aligned}
\frac{\partial}{\partial m}\left(m \sin\frac{\phi}{m} - \left(1 + \frac{m^2 - 1}{6m^2}\phi^2\right)\sin\phi\right) &= \sin\frac{\phi}{m} - \frac{\phi}{m}\cos\frac{\phi}{m} - \frac{\phi^2}{3m^3}\sin\phi \\
&\geqslant \sin\frac{\phi}{m} - \frac{\phi}{m}\cos\frac{\phi}{m} - \frac{\phi^2}{3m^2}\sin\frac{\phi}{m} \\
&= \frac{1}{3}\int_0^{\phi/m} t(\sin t - t\cos t)\,dt \geqslant 0.
\end{aligned}$$

□

3.A.7 A decreasing function

The following technical lemma is of crucial importance in the proof of the monotonicity property in Lemma 3.9.4.

Lemma 3.A.12 *For $\lambda > 0$ and $n \geqslant 6 + 36/\lambda$, the function*

$$\frac{1 - r^n}{1 - r}\exp\left(-\lambda\frac{1 - r^{n/6}}{1 - r}\right)$$

is decreasing with respect to r in the interval $(\exp(-8\lambda/9), 1)$.
Proof: By taking logarithmic derivatives with respect to r, we see that it suffices to prove that

$$\frac{\partial}{\partial r}\log\frac{1-r^n}{1-r} \leqslant \lambda\frac{\partial}{\partial r}\frac{1-r^{n/6}}{1-r}.$$

For the left-hand side, we have

$$\frac{\partial}{\partial r}\log\frac{1-r^n}{1-r} \leqslant \frac{(1-r^n+r^n\log(r^n))}{(1-r)(1-r^n)}$$

(which, after simplification, turns out to be equivalent to the obvious $-\log r^{-1} \geqslant 1-r^{-1}$), and for the right-hand side (without λ and with n replaced by $6n$)

$$\frac{\partial}{\partial r}\frac{1-r^n}{1-r} \geqslant \frac{(1-r^n)(1-r^{(n-1)/2})}{(1-r)^2}$$

(which, after simplification, turns out to be equivalent to the easily derived inequality $n \leqslant r^{-(n-1)/2}+r^{-(n-3)/2}+\cdots+r^{(n-1)/2}$). Therefore, it suffices to prove that

$$\frac{(1-r^n+r^n\log(r^n))}{(1-r)(1-r^n)} \leqslant \lambda\frac{(1-r^{n/6})(1-r^{(n-6)/12})}{(1-r)^2},$$

or, equivalently,

$$\frac{(1-r^{n/6})(1-r^{(n-6)/12})(1-r^n)}{(1-r^n+r^n\log(r^n))(1-r)} \geqslant \frac{1}{\lambda}.$$

We write $s := r^{n-6}$. It is not difficult to show that the function $x \mapsto \frac{(1-x)(1-x^{1/6})}{1-x+x\log x}$ is decreasing for $x \in (0,1)$. Since $s = r^{n-6} \geqslant r^n$, this observation implies that

$$\begin{aligned}\frac{(1-r^{n/6})(1-r^{(n-6)/12})(1-r^n)}{(1-r^n+r^n\log(r^n))(1-r)} &\geqslant \frac{(1-s^{1/6})(1-s^{1/12})(1-s)}{(1-s+s\log s)(-\log r)}\\ &= (n-6)\frac{(1-s^{1/6})(1-s^{1/12})(1-s)}{(1-s+s\log s)(-\log s)}.\end{aligned}$$

Therefore it remains to prove that

$$\frac{(1-s^{1/6})(1-s^{1/12})(1-s)}{(1-s+s\log s)(-\log s)} \geqslant \frac{1}{\lambda(n-6)} \tag{3.129}$$

for $s \in (e^{-8\lambda/9}, 1)$. Let $h(s)$ denote the left-hand side of ((3.129)). The function $s \mapsto h(s)$, for $s \in (0,1)$, equals 0 for $s \to 0^+$ (due to the term $-\log s$ in the denominator), it equals $1/36$ for $s \to 1^-$, it is increasing at the beginning, has a unique maximum at (numerically) $s = 0.00003158\ldots = e^{-10.3629\ldots}$ (with value $h(0.00003158\ldots) = 0.0459021\ldots$), and from there on is decreasing. Since, by assumption, we have $\lambda(n-6) \geqslant 36$, the inequality ((3.129)) will be satisfied on an interval of the form $[y, 1]$, with y depending on λ and n.

We have $h(10^{-12}) = 0.0322464\ldots > \frac{1}{36} = 0.02777\ldots$. Since 10^{-12} is smaller than the place of the unique maximum of $h(s)$, this implies

$$h(s) \geqslant \frac{1}{36} \geqslant \frac{1}{\lambda(n-6)}, \qquad \text{for } s \in (10^{-12}, 1). \tag{3.130}$$

In order to get an estimate for y, we observe that the function $s \mapsto h(s)(-\log s)$, that is,

$$s \mapsto \frac{(1-s^{1/6})(1-s^{1/12})(1-s)}{(1-s+s\log s)},$$

is decreasing for $s \in (0,1)$. Its value at $s = 10^{-12}$ is $0.891\cdots > \frac{8}{9}$. Therefore, we have

$$h(s) \geqslant \frac{8}{9}\frac{1}{(-\log s)}, \qquad \text{for } s \in (0, 10^{-12}).$$

If we now choose $y = e^{-\frac{8}{9}\lambda(n-6)}$, then we have

$$h(s) \geqslant \frac{8}{9}\frac{1}{(-\log s)} \geqslant \frac{1}{\lambda(n-6)}, \qquad \text{for } s \in (y, 10^{-12}).$$

Together with ((3.130)) and the fact that $n \geqslant 7$ by assumption, we have proven ((3.129)) and thus the lemma. □

3.A.8 A cosine inequality

The elementary cosine estimate below is needed in the proofs of Theorems 3.10.2, 3.10.3, and 3.10.4.

Lemma 3.A.13 *For $x \in [-\pi/6, 0]$ and all integers m, we have*

$$|\cos(x - 2m\pi/3)| \geqslant \begin{cases} \frac{1}{2}, & \textit{for } m \equiv 0, 1 \pmod 3, \\ |\cos(\pi/3 - x)|, & \textit{for } m \equiv 2 \pmod 3. \end{cases} \tag{3.131}$$

Proof: We distinguish the congruence classes of m modulo 3. If $m \equiv 0 \pmod 3$, then we have

$$|\cos(x - 2m\pi/3)| = |\cos(x)|. \tag{3.132}$$

The claim on the right-hand side of ((3.132)) is then straightforward to verify. The case where $m \equiv 1 \pmod 3$ can be treated similarly. On the other hand, for $m \equiv 2 \pmod 3$ we actually have

$$|\cos(x - 2m\pi/3)| = |\cos(\pi/3 - x)|.$$ □

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